

**CP1****Improving Ultimate Convergence of An Augmented Lagrangian Method**

Optimization methods that employ the classical Powell-Hestenes-Rockafellar Augmented Lagrangian are useful tools for solving Nonlinear Programming problems. Their reputation decreased in the last ten years due to the comparative success of Interior-Point Newtonian algorithms, which are asymptotically faster. In the present research a combination of both approaches is evaluated. The idea is to produce a competitive method, being more robust and efficient than its "pure" counterparts for critical problems. Moreover, an additional hybrid algorithm is defined, in which the Interior Point method is replaced by the Newtonian resolution of a KKT system identified by the Augmented Lagrangian algorithm.

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**CP1****Augmented Lagrangian Algorithm with Recursive Trust-Region Method: Application to Optimal Control Problems with Equality Constraints**

In this talk, preliminary numerical results of augmented Lagrangian algorithm ALDISCR by Sartenaer and Sachs are presented. This algorithm is tailored for infinite-dimensional optimization problems with equality constraints, like optimal control problems. ALDISCR considers a sequence of discretized augmented Lagrangian subproblems with dynamically determined discretization levels to ensure global convergence. An application of the recursive multiscale trust-region method from Gratton, Sartenaer and Toint within this framework to solve the subproblems is also proposed and discussed.

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**CP1****On the Use of Iterative Methods for Solving Linear Equations in Nonlinear Optimization**

Solving linear equations is an important step in many methods for nonlinear optimization, e.g., interior methods. In some cases, the matrices are symmetric and ill-conditioned. This may be due to e.g. symmetrization of the linear equation in an interior method or ill-posedness of an inverse problem. We discuss the behavior of conjugate-gradient type methods on such ill-conditioned linear equations.

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**CP1****A Second-Derivative SQP Method for Nonconvex Optimization Problems with Inequality Constraints**

We consider a second-derivative  $\ell_1$  sequential quadratic programming trust-region method for large-scale nonlinear non-convex optimization problems with inequality constraints. Trial steps are composed of two components; a Cauchy globalization step and an SQP correction step. A single linear artificial constraint is incorporated that ensures non-accident in the SQP correction step, thus "guiding" the algorithm through areas of indefiniteness. A salient feature of our approach is feasibility of all subproblems.

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**CP2****A Multilevel Algorithm for Inverse Problems with Bound Constraints**

We present a provably scalable algorithm for solving a class of inverse problems in the presence of bound constraints. Previous analysis proved that the associated unconstrained problems can be solved efficiently using specially designed multilevel preconditioners. An extension of that technology is combined with a semismooth Newton method to show that the bound-constrained inverse problem can be solved at a cost that is decreasing with increasing resolution relative to that of the forward problem.

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**CP2****An Interior Method for Computing a Trust-Region Step**

We consider methods for large-scale unconstrained optimization based on finding an approximate solution of a quadratically constrained trust-region subproblem. The solver is based on sequential subspace minimization with a modified barrier "accelerator" direction in the subspace basis. The method is able to find solutions of the subproblem to any prescribed accuracy. Numerical results will be presented. This is joint work with Philip Gill and Joshua Griffin.

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## CP2

### Modified Line Search for High Dimensional Functions Optimization

This paper proposes a modified line search method which makes use of partial derivatives and re-starts the search process after a given number of iterations by modifying the boundaries based on the best solution obtained at the previous iterations. Performance of the proposed algorithm is compared with genetic algorithm and particle swarm optimization for functions having up to 10,000 dimensions for which line search clearly outperforms the other methods.

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## CP2

### A Safeguarded Line Search Algorithm Using Trust Region Approach

In this talk, we present an hybrid algorithm for unconstrained nonlinear optimization which combines line search and trust region strategies. More precisely, the proposed method implements a line search technique but allows the exploitation of directions of negative curvature by switching to a trust region approach when such a direction is encountered. We detail an adaptation of the Steihaug-Toint conjugate gradient algorithm and report some preliminary numerical results.

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## CP2

### Efficient Curve Detection Using the Gauss-Newton Method

The detection of geometric primitives, like lines, circles or ellipses, in an image plays a crucial role in many computer vision applications. In this talk, we present a new approach to such problem using a Low-Order-Value Optimization model that can be tackled by variations of the Gauss-Newton method. The proposed model is robust to noise and very efficient to find patterns described by many parameters. We present extensive performance comparisons to many classical algorithms.

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## CP3

### Goal Oriented Adaptivity and Multilevel Techniques for Shape Optimization with Inviscid Flows

We present a continuous adjoint approach to shape optimization for turbulent flows modelled by the incompressible instationary Navier-Stokes equations. After introducing the analytical adjoint calculus in the presence of stabilization terms, we will focus on adaptivity based on a goal oriented error estimator and multilevel optimization with inexact trust-region SQP techniques. Numerical results will be presented.

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## CP3

### A Newton-Multigrid Method for One-Shot Pde-Constrained Optimization

We present a Newton-Multigrid method for the fast solution of PDE-constrained optimization problems. Applying an inexact Newton method to the nonlinear optimality system yields a sequence of quadratic optimization problems. An efficient preconditioner is mandatory for the coupled iterative solution of these ill-conditioned and indefinite systems. To this end, a multigrid algorithm together with appropriate smoothing iterations is developed. We discuss different relaxation methods and their properties for a variety of optimal control problems.

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### CP3

#### The Minimization of an $L^\infty$ -Functional Subject to an Elliptic PDE and Pointwise State Constraints

We study the optimal control of a maximum-norm objective functional subjected to an elliptic-type PDE and point-wise state constraints. The problem is transformed to a problem where the on-differentiable  $L^\infty$ -norm in the functional will be replaced by a scalar variable and additional state constraints. This problem is solved by barrier methods. We will show the existence and convergence of the central path for a class of barrier functions. Numerical experiments complete the presentation.

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### CP3

#### Numerical Methods for Inverse Transport Problems and Applications

We consider the problem of reconstructing physical parameters ( $\Sigma(\mathbf{x})$  and  $\Sigma_s(\mathbf{x})$ ) in the radiative transport equation:

$$\theta \cdot \nabla u(\mathbf{x}, \theta) + \Sigma(\mathbf{x})u(\mathbf{x}, \theta) = \Sigma_s(\mathbf{x}) \int_{\mathbb{S}^{d-1}} \mathbf{k}(\theta \cdot \theta') u(\mathbf{x}, \theta') d\mu(\theta')$$

$$u(\mathbf{x}, \theta) = \mathbf{g}(\mathbf{x}, \theta), \quad (\mathbf{x}, \theta) \in \Gamma_-$$

where  $\Gamma_- \equiv \{(\mathbf{x}, \theta) \in \partial\Omega \times \mathbb{S}^{d-1} \text{ s.t. } \theta \cdot \nu(\mathbf{x}) < 0\}$ .  $\Omega \in \mathbb{R}^d$  is the domain of interest and  $\mathbb{S}^{d-1}$  is the unit sphere in  $\mathbb{R}^d$ . We solve those inverse problems numerically using the framework of PDE-constrained optimization. Two specific applications of those inverse problems are considered: optical tomography and incoherent imaging in random media. Numerical examples based on synthetic and experimental data will be presented. Main references are: [1] Frequency domain optical tomography based on the equation of radiative transfer, SIAM J. Sci. Comput., 28, 1463-1489, 2006. [2] Transport-based imaging in random media, submitted, 2007. [3] Experimental validation of a transport-based imaging method in highly scattering environments, Inverse Problems, 23, 2527-2539, 2007.

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### CP3

#### PDE-Constrained Optimization in Nuclear Reactor Designs.

In this study we will demonstrate how to use PDE-constrained optimization for nuclear reactor design. The problem is how to optimize the heat source such that the wall (clad) temperature will not exceed the melting temperature. Hence, it is inequality constrained optimization. Two approaches are proposed, i.e. inverse source and exterior penalty functional. Then, we compare the methods to each other. Our conclusion is that the two techniques are similar in terms of the optimized heat sources and the

temperatures.

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### CP4

#### Solution of Integer Bilevel Linear Programming Problems

Input your abstract, including TeX commands, here. The abstract should be no longer than 75 words. Only input the abstract text. Don't include title or author information here.

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### CP4

#### An Optimization Approach to Radio Resource Management.

In this talk we consider a radio cellular system in which each cell manages the radio resources for its own users and services. The radio resources are orthogonal within each cell, e.g. Orthogonal Frequency Division Multiple Access (OFDMA). However, inter-cell interference is an issue if nearby cells use the same resource simultaneously. The scheduling problem of the system is posed as a mathematical optimization problem. Various problem formulations and different solution methods will be discussed.

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### CP4

#### A Two-Phase Approach for a Trumper Ship Scheduling Problem

We present two-phase approach for solving a trumper ship scheduling problem in Japan. Firstly, a few transportation orders are aggregated into one order. Secondly, we solve routing problem by set partitioning approach. It involves many columns so that column-generation method is applied. Because of the aggregation in the first-phase, the subproblems become time-dependent shortest path problems and are easily solved by labeling algorithm. Our numerical results show that the proposed algorithm is effective.

tive.

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#### CP4

##### **Discrete Bilevel Programming: Applications and Solution**

A bilevel programming problem consists of an upper level optimization problem whose set of feasible solutions depends on the set of optimal solutions of a lower level problem. Our focus is on discrete bilevel programming problems where the lower and/or the upper level problems have binary variables. We propose to reformulate the discrete problem and solve it using a global optimization approach. Numerical results on a biofuel production application will be presented.

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#### CP5

##### **Applications of Semidefinite Programs with Log-Determinant Terms**

The Tsuchiya-Xia's primal-dual path-following interior-point algorithm for SDPs with weighted log-determinant was implemented in the SDPA. These problems often appear in statistics related problems. We review the basic features of Tsuchiya-Xia's algorithm, and we present applications in quantum tomography and data assimilation where we need to solve several small SDPs or a very large SDP with weighted log-determinant.

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#### CP5

##### **Large Scale Semidefinite Programming Arising from Chemistry**

The electronic structure of ground state of atoms and molecules are very important in chemistry and physics. The basic equation is Schroedinger equation, but it becomes very hard to solve when the system becomes larger. We use the second-order reduced density matrix (2-RDM) as basic variable which is simpler, instead of complicated wave function. This method is formulated as semidefinite programming of arbitrary size. In this session, we present

some recent results of this method.

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#### CP5

##### **New Sdp Relaxations for Quadratic Assignment Problems Based on Matrix Splitting**

QAPs are known to be among the hardest discrete optimization problems. In this talk we propose new SDP relaxations for QAPs based on matrix splitting technique. Our new SDP relaxation has a smaller size compared with other SDP relaxations in the literature and can be solved efficiently by most open source SDP solvers. Experiments show that rather strong bounds can be obtained for large scale QAP instances up to  $n=150$ . Further simplification and improvement of our new model based on the data structure in the underlying QAP will be discussed as well.

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#### CP5

##### **Matrix Convex Functions and Optimization**

In this talk, we discuss various differentiation rules for general smooth matrix-valued functions, and for the class of matrix convex (or concave) functions first introduced by Löwner and Kraus in the 1930s. For a matrix monotone function, we present formulas for its derivatives of any order in an integral form. Moreover, for a general smooth primary matrix function, we derive a formula for all of its derivatives by means of the divided differences of the original function. As applications, we use these differentiation rules and the matrix concave function  $\log X$  to study a new notion of weighted centers for Semidefinite Programming (SDP). We show that, with this definition, some known properties of weighted centers for linear programming can be extended to SDP. We also show how the derivative formulas can be used in the implementation of barrier methods for optimization problems involving nonlinear but convex matrix functions. This talk is based on a joint paper with Jan Brinkhuis and Tom Luo.

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#### CP6

##### **Minimum Area Enclosing Ellipsoidal Cylinder Problem**

Given an arbitrary set  $A \in R^n$  and an integer  $k : 0 \leq k \leq n$ , we are interested in finding an ellipsoidal cylinder, centered at the origin, such that its intersection with the subspace  $\{y \in R^n : y_{k+1} = \dots = y_n = 0\}$  has mini-

imum area. This problem is referred to as the Minimum-Area Enclosing Ellipsoidal Cylinder (MAEC) problem. We show that MAEC and its dual can be written as convex problems, and present a Frank-Wolfe type algorithm with away steps. This algorithm finds an  $\epsilon$ -approximate solution in  $O(k(\log k + \log \log m + \epsilon^{-1}))$  iterations under some assumptions where  $|A| = m$ . We present some computational results and discuss local convergence properties of the algorithm.

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### CP6

#### Dual Problems of Extremal Volume Ellipsoids

The minimum (maximum) volume ellipsoid containing (contained in) a convex body in  $R^n$  is an important problem having applications in optimization, statistics, data mining and control theory, among others. As the numerical computation of these ellipsoids is needed in all the applications mentioned, the study of the dual problems become crucial. In this talk, we focus on the duals of the extremal volume ellipsoids utilizing semi-infinite programming duality.

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### CP6

#### A Simple Variant of the MTY-PC Algorithm and Its Objective-Function-Free Polynomial-Time Convergence for Bounded LPs

We analyze a simple variant of the Mizuno-Todd-Ye predictor-corrector (MTY-PC) algorithm for LP. The modified algorithm utilizes a scaling-invariant two-layered least squares step which naturally arises when a scaling-invariant finite termination procedure is considered. Under the assumption that the feasible region is bounded, we prove polynomial-time complexity of the algorithm that does not depend on the objective function. Our result yields a practical strongly polynomial-time complexity algorithm for the feasibility problem of combinatorial LPs.

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### CP6

#### A Cutting Plane Method for Semi-Infinite Linear Programming

We present a cutting plane algorithm for semi-infinite linear programming. At each iteration a relaxation of the original problem is formed that contains a finite number of constraints. A point in the vicinity of the central path of this problem is computed and violating constraints are identified at this point. Then the relaxation is updated by adding the new constraints and the barrier parameter is simultaneously reduced. We show that after a finite number

of iterations an  $\epsilon$ -optimal solution is obtained.

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### CP7

#### Smoothed Monte Carlo in Robustness Optimization

Robustness is seen as the probability mass of a design dependent set. An alternative for Monte Carlo is Smoothed Monte Carlo (SMC) estimation. The idea is to add a smoothing term to the MC estimation function resulting into continuity in interesting design points. It is proven that the resulting estimate function is continuous in such points, arbitrarily close to the MC estimator and facilitates the use of standard optimisation algorithms. The whole is illustrated numerically.

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### CP7

#### A New Methodology for Evacuation Modelling Analysis Using Numerical Optimisation Techniques

This work intends to demonstrate how optimization techniques can be applied to evacuation analysis to determine optimal configurational layout. In particular we present a methodology that combines the numerical techniques of Design of Experiments, Response Surface Models and numerical optimization with the buildingEXODUS evacuation simulation tool. The proposed methodology is demonstrated through an example involving a square room with two exits. The methodology is applied to this problem and the optimal exit configuration is determined.

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### CP7

#### Pattern Search Algorithms for Circuit Design Optimization

This research work presents three Pattern Search Algorithms, Mesh Adaptive Direct Search, Generalized Pattern Search and Particle Swarm Pattern Search, on two circuit design optimization problems: the parameter extraction of an inductor circuit model and the problem of device sizing of an Operational Transconductance Amplifier. We compared these optimization algorithms in terms of quality and robustness of the solutions and in terms of the computational effort needed to compute them.

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### CP7

#### Maximin Latin Hypercube Designs

Latin hypercube designs (LHDs) play an important role in approximating computer simulation models. To obtain good space-filling properties, the maximin criterion is used, i.e., the objective is to obtain an LHD of  $n$  points in  $k$  dimensions with maximum separation (minimal) distance. We give bounds for the separation distance of LHDs and give construction methods for approximate maximin LHDs. These results among others use mixed integer programming, a graph covering problem, and orthogonal arrays.

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### CP7

#### A Method for Simulation Based Optimization Using Radial Basis Functions

We propose an algorithm for the global optimization of expensive and noisy black box functions using response surfaces based on radial basis functions (RBFs). To handle noise, a method for RBF-based approximation is introduced. New points are selected to minimize the total model uncertainty weighted against the surrogate function value. We present an extension of the algorithm to multiple objectives. Numerical results on analytical test functions and simulations show promise.

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### CP8

#### Computing Optimal Trajectories for Low-Energy Spacecraft Transfers

The number of spacecraft missions in which low-thrust propulsion systems are applied for orbit transfer and interplanetary travel has been rapidly growing in recent years, because this technology has proven to enable missions that would otherwise not be feasible. The author will present a number of examples of large trajectory problems related to low-energy and low-thrust transfers that have been op-

timized with NLP solvers.

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### CP8

#### Optimal Control of Delay Systems with Constraints

We consider optimal control problems with constant delays in state and control variables under mixed control-state inequality constraints. First order necessary optimality conditions are presented and as well as a numerical method based upon discretization techniques and non-linear programming. The theory and the proposed numerical method are illustrated by applications taken from biomedicine and chemical engineering in order to apply the proposed algorithm and to compare the computed results with the theory.

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### CP8

#### On a Special Constraint in Least-Time Path Problems.

We investigate a fairly general class of problems, that use constraints related to prescribed speed. Related problems arise naturally from considerations of conservation of energy, as in the brachistochrone. No such assumptions are used here. The same equations for the parameter used to describe the constraint, under a slight generalization, gives that of curves of fixed rhumb. Based on similar ideas, we try to provide the structure of a solution for the simplest of such constraints on a simple surface. We show a trivial, non-smooth solution, which might eventually be used in the construction of a numerical solver.

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### CP8

#### Optimal Multi-Drug Control of a Delay-Differential Model of the Immune Response

Optimal control problems with time delays in state or control variables and control-state inequality constraints are discussed in the foregoing talk by Goellmann et al. In this talk, we apply the Minimum Principle and the numerical methods to the optimal control model of the immune response (R. Stengel et al., Optimal control of innate immune response, OCAM 23, 91-104, 2002). Here, only non-delayed equations are considered, therapeutic agents

are treated separately and the objective function is assumed to be quadratic in control. In this talk, we discuss optimal multi-drug control protocols for non-delayed and delayed equations and compare optimal solutions for objective functionals of  $L^2$  and  $L^1$  type. Furthermore, we present state-constrained and time-optimal solutions. We consider optimal control problems with control appearing linearly. This class of control problems is well studied for ordinary differential equations. Here, the optimal control is found to be a combination of bang-bang and singular subarcs, where the junction points between subarcs are determined by an associated switching function. The purpose of this talk to present several control problems for elliptic and parabolic equations which exhibit bang-bang and singular controls and illustrate phenomena similar to those in the ODE case.

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### CP8

#### On Convergence of Regularization Methods for Parabolic Optimal Control Problems with Pointwise Control and State Constraints

Pointwise state constraints present a challenge for the analysis as well as the numerical treatment of optimal control problems, since associated Lagrange multipliers can generally only be expected to exist in the space of regular Borel measures. In the past, different regularization strategies have been developed in order to avoid this difficulty. They have, however, mainly been considered for pure state constraints or unilateral control and state constraints. Here, we focus on semilinear parabolic optimal control problems governed by bilateral pointwise state and control constraints. Exemplarily, we apply Lavrentiev regularization and present some difficulties associated with the given constraints. We rely on an additional assumption on the structure of the problem, namely a separation condition on the active sets, and show convergence for vanishing regularization parameter as well as a local uniqueness result for local optima based on second order sufficient conditions.

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### CP9

#### Practical Methods for Constrained Oilfield Optimization

Oilfield optimization problems are expensive to compute and typically have constraints, possibly nonlinear, on the control parameters. Such complex problems might not have derivatives of the objective function available, because they are impossible to obtain analytically or too expensive to evaluate numerically. Unfortunately, most derivative-free optimization algorithms treat unconstrained problems. In this study, we discuss the efficient use of penalty and lexicographic comparison based methods to optimize oil

production under nonlinear physical constraints.

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### CP9

#### Systems of Systems Optimization Formulations with Application to Aircraft Selection and Design

We examine optimization issues for systems of systems; these include the tradeoff of degree of central authority vs. component autonomy, and predictive modeling of components input-output responses. We illustrate these optimization concepts on the problem of simultaneous product design and fleet mix optimization problem. Results will be given for an aircraft selection exercise, including extension to determining the best aircraft family, and to problems having a mix of continuous and categorical variables.

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### CP9

#### Improving the Method of Seed Generation for a Route Optimization Software Package

Quantm provides software for road and rail infrastructure planning. A service Quantm provides is unseeded optimization, whereby 50 routes are produced from scratch, requiring the generation of 50 different seed routes from a continuous space. The method for the generation of the seeds by constructing a network over the land surface and using shortest path algorithms is presented, along with two different attempts to improve the quality of results produced by this method.

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### CP9

#### Optimization of Satellite Coverage

This project is concerned with satellite-based environmental observation. For an effective monitoring of environmental activities by a satellite, it is the main goal to achieve maximum coverage throughout a short period of time. Due to technical restrictions of the satellite hardware, it is only possible to use the camera for a limited time period per orbit, while rotating around the Earth. The main goal is

to determine the time intervals for which the coverage with respect to given target areas is maximized and the restrictions such as contact to ground stations are satisfied. To achieve a continuous objective function for the sequential quadratic programming method, the coverage is modelled by polygons integrated on a sphere. For acceptable computing times, special investigations had to be made in order to achieve fast gradient computations.

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### CP9

#### Forward Swept Wing Optimization by Using the Genetic Algorithm

This work is about forward swept wing (FSW) design problem for reducing the optimization time and cost. Dynamic mesh technique was used in the design of a transonic FSW by coupling it with Genetic Algorithm. It is observed that the drag coefficient can be reduced by 15 percent while the lift coefficient close to the design value determined at the beginning as a design constraint. The results are also compared to backward swept results.

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### CP10

#### Complexity Reduction of Calibration Problems in Numerical Finance

The pricing of derivatives has gained considerable importance in the finance industry and leads to challenging problems in numerical optimization. We focus on the numerical solution of a stochastic model for option prices. In particular, we are concerned with the calibration of these models to real data, which leads to large scale optimization problems. We consider the numerical solution of these optimization problems and give some indication how to reduce the complexity of these problems.

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### CP10

#### Models and Algorithms for Stackelberg Games with Incomplete Information

Stackelberg games, where one player, the leader, selects its action first and the second player decides its optimal strategy knowing the actions of the leader is a natural problem for various security domains. This framework however assumes the leader has an accurate model of the adversary. In this work we have developed efficient mixed-integer programs and algorithms to solve situations where there is imperfect information about the adversary, its reward structure, or decision process.

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### CP10

#### A Numerical Method for Stochastic Control with Applications to Finance

We solve a series of stochastic control problems on a diffusion process using a combination of Ito calculus, martingale theory and linear programming. With sparse matrix techniques, a manageable number of constraints and using the MOSEK solver embedded into Matlab, our methodology provides for a quick and easy way to solve this type of stochastic control problem. We apply the numerical methodology to a series of problems in corporate finance, yielding some interesting results.

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### CP10

#### Information Relaxations and Duality in Stochastic Dynamic Programs

We describe a dual approach to stochastic dynamic programming: we relax the constraint that the chosen policy must be temporally feasible and impose a penalty that punishes violations of temporal feasibility. We describe the theory underlying this dual approach and demonstrate its use in inventory models and option pricing models.

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### CP10

#### Index Policies for Discounted Bandit Problems with Availability Constraints

We study a generalization of the multi-armed bandit problem where arms are not always available. We prove the non-existence of an optimal index policy and propose the so-called Whittle index policy by formulating the problem as a restless bandit problem. The index policy cannot be dominated uniformly by any other index policy over the entire class of bandit problems considered here, and is numerically shown to be near-optimal.

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### CP11

#### Globalization of Primal-Dual Methods for Nonlinear Programming

We propose a new globalization strategy for primal-dual methods in nonlinear programming. Our technique relaxes the usual requirement of solving the barrier problem with a precision of the same order as the barrier parameter. We show that the full Newton step is asymptotically ac-



cepted and that linear or superlinear convergence occurs when the barrier parameter goes to zero linearly or superlinearly. Numerical experiments are presented.

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### CP11

#### A Graph-Based Decomposition Method for Quadratic Separable Programs

A graph is derived based on the QSP model. KKT complementarity conditions are used in order to decide how the graph has to be traversed in the solution process. Also, a decomposition strategy is applied in order to divide the problem into subproblems by "weakening" the links which connect the variables. This has the effect to take into account those links to complete their gradient but are disregarded in the propagation to solve the system.

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### CP11

#### Null-Space Primal-Dual Interior-Point Methods for Nonlinear Programs with Strong Convergence Properties

We consider a class of primal-dual interior-point methods for solving nonlinear optimization problems with general inequality and equality constraints. The methods approximately solve a sequence of equality constrained barrier subproblems by computing a range-space step and a null-space step in every iteration. The  $\ell_2$  penalty function is taken as the merit function. Under very mild conditions on range-space steps and approximate Hessians, without assuming any regularity, it is proved that either all limit points of the iterate sequence are Karush-Kuhn-Tucker points of the barrier subproblem and the penalty parameter remains bounded, or there exists a limit point that is either an infeasible stationary point of minimizing the  $\ell_2$  norm of violations of constraints of the original problem or a Fritz-John point of the original problem. Locally, we prove that by suitably controlling the exactness of range-space steps, selecting the barrier parameter and Hessian approximation, the methods generate a superlinearly or quadratically convergent step.

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### CP11

#### Solving Continuous Nonlinear Optimization Via Constraint Partitioning

We present a novel constraint-partitioning approach for nonlinear optimization. In contrast to previous work, our approach is based on a new exact penalty theory and can handle global constraints. We employ a hyper-graph partitioning method to recognize the problem structure. We prove global convergence under assumptions that are much more relaxed than previous work and solve problems as large as 40,000 variables that other solvers such as IPOPT cannot solve.

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### CP12

#### On Automatic Differentiation for Optimization

Automatic problem setup, e.g., by a modeling language, helps promote use of optimization algorithms. For some nonlinear optimization algorithms, accurate derivative computations are essential. This talk reviews use of automatic differentiation as an ingredient in optimization problem setup, touching on implementation techniques, gradient and Hessian-vector products, and experience both with facilities connected with the AMPL modeling language and with Sacado, a Sandia package for automatic differentiation of C++ codes.

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### CP12

#### Globally Convergent Three Term Conjugate Gradient Methods for Large-Scale Unconstrained Optimization Problems

In this talk, we deal with a new three term conjugate gradient method for solving large-scale unconstrained optimization problems. It always generates sufficient descent direction independently of line searches. We consider a sufficient condition for the global convergence of the proposed method within the line search strategy. Moreover, we propose a new method within this strategy, and establish its global convergence. Finally, some numerical results of the proposed method are given.

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### CP12

#### A Class of Methods Combining L-BFGS and Truncated Newton

We present a class of methods which is a combination of the limited memory BFGS method and the truncated New-

ton method. Each member of the class is defined by the (possibly dynamic) number of vector pairs of the L-BFGS method and a dynamic forcing sequence of the truncated Newton method. We exemplify with a scheme which makes the hybrid method perform like the L-BFGS method far from the solution, and like the truncated Newton method close to the solution. Numerical results indicate that the hybrid method usually performs well if one of its parent methods performs well.

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### CP12

#### Limited Memory Bfgs Updating in a Trust-Region Framework for Large-Scale Unconstrained Problem

In this talk we show that the limited memory updates to the Hessian approximations can also be applied in the context of a trust-region algorithm. At each iteration, an explicit quasi-Newton step is computed. If it is rejected, then we compute the solutions for trust-region subproblem with the trust-region radius smaller than the length of quasi-Newton step. The key to this observation is the compact form of the limited memory updates derived by Byrd, Nocedal, and Schnabel. Numerical results will be discussed.

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### CP12

#### Nonlinear Conjugate Gradient Methods with Structured Secant Condition for Nonlinear Least Squares Problems

In this talk, we deal with conjugate gradient methods for solving nonlinear least squares problems. By combining the idea of Dai-Liao's conjugate gradient method and the structured secant condition used in structured quasi-Newton methods, we propose conjugate gradient methods that make use of the structure of the Hessian of the objective function. The present methods are shown to be globally convergent under some assumptions. Finally, numerical results are reported.

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### CP13

#### Sensitivity to Observations in Model-Constrained Optimization

The sensitivity of the least-squares state estimation to observational data is considered in the context of nonlinear model-constrained optimization. The sensitivity equations are derived from the first order optimality conditions and a second order adjoint model is used to provide Hessian matrix information. Practical implementation for large-scale systems and order reduction are discussed. Numerical results and sensitivity to time-space distributed data are presented with a two-dimensional shallow-water model.

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### CP13

#### A Convex Output Least-Squares for the Elliptic Inverse Problems

The coefficients in a variety of linear elliptic partial differential equations can be estimated from interior measurements of the solution. This talk will focus on the estimation of the coefficients in an abstract variational equation. The main motivation behind the study of this inverse problem is to identify Lamé coefficients in the system of linear elasticity. Recently, interesting applications, such as elasticity imaging, have sparked a new interest in this problem. More specifically, it is possible, using ultrasound, to measure interior displacements in human tissue (for example, breast tissue). Since cancerous tumors differ markedly in their elastic properties from healthy tissue, it may be possible to discover and locate tumors by solving an inverse problem for the Lamé parameters. Recently, we introduced a new modified output least-squares formulation in an abstract setting and proved its convexity. This circumvents a serious deficiency of classical output least-squares functional of being nonconvex in general. The abstract formulation is general enough to be able to recover the main features of the total variation regularization. (The use of total variation regularization allows the identification of discontinuous coefficients.) The main emphasis of the talk will be on the stability issues for the modified output least-squares functional. Two kinds of stability results will be presented. The first approach relies on a certain embedding properties of the spaces involved along with some functional analytic manipulation of the functional. The second approach will make use of some abstract results from optimization theory. Several numerical examples will be presented to show the feasibility of the approach.

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### CP13

#### Constrained Orthogonal Distance Regression to Compute Parameters in a Lotka-Volterra System

### of Differential Equations

We present an application which is modeled as a system of differential equations. A finite number of values for the curves that solve the system are available. The target is to compute parameters on the system in order to obtain curves that are as close as possible to the observed data. Since the observed data may have noise in the primal variable, we propose an orthogonal distance regression scheme to compute such parameters.

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### CP13 Parameter Identification with a Blood Pressure, Blood Flow Model

We present a compartmental model for blood pressure and blood flow in the human body. The resulting ODE system contains many physiological parameters specific to the subject that are difficult to measure directly. We apply cutting edge optimization techniques to identify parameter values that cause the ODE solution to fit data collected noninvasively. Care is taken to determine the subset of model parameters that can be identified reliably.

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### CP14 Algorithms for Robust Shortest Path Problem

In the context of robust discrete optimization where data uncertainty is modeled by values belonging to closed intervals, the Bertsimas and Sim approach and the minimax regret model are the main known methodologies. We implemented algorithms for solving robust shortest path in networks instances using the two methodologies mentioned.

Interesting results were obtained when we analyzed exact and approximate solutions and the possible comparison for these models.

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### CP14 Throughput Optimization in Mobile Backbone Networks

This work develops techniques for throughput optimization in a hierarchical distributed sensing architecture known as a mobile backbone network. We develop a novel technique based on mixed integer linear programming, which leads to a dramatic reduction in computation time compared to existing optimal algorithms. Furthermore, we describe a new polynomial-time approximate solution to this problem. We also formulate natural extensions to the mobile backbone network problem and describe exact and approximate solutions for these extensions.

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### CP14 Fully Polynomial Time Approximation Schemes for Time-Cost Tradeoff Problems in Series-Parallel Project Networks

We consider the deadline problem and budget problem of the nonlinear time-cost tradeoff project scheduling model in a series-parallel activity network. We develop fully polynomial time approximation schemes for both problems using K-approximation sets and functions, together with series and parallel reductions.

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### CP14 Separable Spanning Trees Optimization for Com- munication Networks Reliability

This paper presents a class of iterative parametric dynamic

programming models devoted to networks reliability. Multiobjective optimization is invoked as a separation strategy and the optimal solution is obtained by a multilevel strategy. Lower level weighted power Lagrangian problem is solved using dynamic programming. Upper level adjusts the value of the weighting vector in the weighted power Lagrangian problem. The solution process is iterated until the optimal solution of the reliability optimization problem is found.

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#### CP14

##### **Integer Programming for Optimization of a Large Transportation Network**

Given a set of processing centers, flows of resources, and the existing multimodal transport network, we aim to optimize the resource delivery in the terms of time, cost, and the number of transshipping. The restrictions may concern times of delivery, predefine delivery routes and vehicles to be used. We describe an integer programming approach to this problem and present some techniques for size reduction. Computation on the transportation network of Russia will be reported.

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#### CP15

##### **A New Conic Solver for a Class of Structured Convex Problems**

We present a new conic solver based on interior-point methods that can solve a large class of convex problems, in particular convex problems involving powers, exponentials and logarithms, and report numerical results. We also present a preliminary modelling environment suitable for formulating and feeding problems to this solver. A given convex problem is transformed - if possible - into a structured conic format based on the one-parameter family of power cones (including its limit).

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#### CP15

##### **A Symmetric Primal-Dual Algorithm for Conic Optimization Based on the Power Cone**

The power cones form a family of convex cones that allow the formulation of a large class of convex problems (including linear, quadratic, entropy, sum-of-norm and geometric optimization) into a unified structured conic format. We introduce a primal-dual interior-point algorithm for the this class of problems, which focuses on preserving the perfect symmetry between the primal and dual sides of the problem (arising from the self-duality of the power cone).

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#### CP15

##### **Fine Tuning Nesterov's Optimal Descent Method**

Each iteration of Nesterov's algorithm for minimizing a convex  $C^1$  function starts by computing a constant  $\alpha_k$  dependent on a Lipschitz constant  $L$  for  $f'(\cdot)$ . Then a point  $y^k$  is computed, from which a steepest descent step determines the next iterate  $x^{k+1}$ . We modify the process by first computing  $y^k$  and  $x^{k+1}$  independent of  $L$ , and then an "optimal" value of  $\alpha_k$ . The complexity obtained by Nesterov is kept and the performance improves in test problems.

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#### CP15

##### **An Improved VU-Algorithm for Partly Smooth Minimization**

A recent VU-algorithm for minimizing convex functions implicitly exploits any underlying partly smooth function structure. It follows a "primal-dual track" superlinearly, by alternating U-Newton-predictor-steps with V-corrector-steps. A prox-parameter-dependent bundle subroutine constructs a V-model of the function using past subgradients in order to generate the required U-gradients. This talk describes an improved version that preserves global convergence while incorporating a new strategy for prox-parameter variation which allows this parameter to grow without bound. Results of numerical experiments are presented for validation.

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#### CP15

##### **Distance Function and Infeasible-Start Interior-Point Method**

We formulate the convex program into a unconstrained problem and solve by an infeasible-start interior-point method. The method can be started from any interior-point. We give a new distance function which can be used to study complexity of the method for feasible and infeasible cases. We also give rounding error analysis and design an accurate numerical method for the method. Numerical examples are provides.

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**CP16****Variational Analysis of Robust Regularization**

In continuous optimization, a solution can fail to be robust due to inaccuracies in measurement and implementation. To address robustness in a minimization problem, we consider the maximum of a function over a bounded set and its translations over the domain. This method has regularizing properties, especially for semi-algebraic functions. The relationship between calmness and Lipschitz continuity in Variational Analysis generalizes robust regularization to set-valued maps as well.

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**CP16****Stability Assessment of Partially Identified System Using LMI Optimization**

Vinnicombe Generalized Stability Margin (GSM) provides powerful tool for robustness assessment of control system stability. However, it requires frequency response estimation of both the plant and controller of the system. A method is proposed for computation of GSM using only frequency response of joint “plant-controller” or “controller-plant” block. If the number of system inputs greatly exceed the number of outputs or vice versa, the method allows to reduce expenses spent on system identification.

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**CP16****Robust Optimization and Problem Robustness**

Robust Optimization has been an important approach in recent years, with several emerging applications. Robust solutions are protected from data variation, but the change in the robust solution with respect to the nominal solution is related to the robustness and well posedness of the model itself. In this work we show some results relating both concepts as well as some studies on simulated problem as well as some real Supply Chain Management problems.

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**CP17****Reliability Optimization of Communication Networks Using Genetic Algorithm**

Evolutionary algorithms often have to solve optimization problems in the presence of a wide range of uncertainties.

A new genetic model is considered to study the reliability optimization in a linear consecutively connected system (LMCCS) by allocating multi state elements. A LMCCS consists of  $(N+1)$  linear ordered positions.  $M$  statistically independent multi state elements with different characteristics are to be allocated to the first  $N$  positions. Each element can provide a connection between the position to which it is allocated and next few positions. The system is reliable if the first position (source) is connected with the  $(N+1)$ th position (sink) by means of suitable allocation of the multi state elements in various in between positions (workstations). This means that the signal can be transmitted with out interruption from the source to the sink. As further extension in the proposed genetic model, reliability optimization is attempted in LMCCS by allocating Multi-state Elements in various workstations by considering the adverse effects of noise in signal transmission. The reliability of LMCCS is obtained using Universal Generating Function technique. The optimal allocation is obtained by means of Genetic Algorithm. For the one-to-one allocation problem, when the permutation crossover is used, it reduces the complexity of the problem and also yield better result compared to all the existing results.

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**CP17****Optimization Population-Based Algorithms for High-Performance Analog Circuits**

This paper tackles the Integrated Circuit (IC) design by population-based algorithms. The following real-life circuits, *RF Low Noise Amplifier*, *Leapfrog Filter*, and *Ultra Wideband LNA*, were selected as test bed. The proposed algorithms, ADVACED-NSGAI and OPTIA, were shown to produce acceptable and robust solutions in the tested applications, where state-of-art algorithms, circuit designers and commercial techniques failed. The results show significant improvement in all the chosen IC design problems.

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**CP17****Automatic Layout Optimization of Power Mosfets Using An Effective Population-Based Algorithm**

The robustness of high-voltage discrete power MOSFETs strictly depends on the topology of the layout device; the optimization task is to minimize the maximum temperature reached by the device. A complete exploration of the solution space is impossible due the huge number of configurations. The designed population-based algorithm is able to find sub-optimal topologies, that improves the performance of the device of 27% respect the one proposed by designers and significantly outperforms state-of-art optimization algorithms.

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### CP17 Heuristically Evolving Populations Broaden Problem Understanding

Population-based evolutionary heuristics can seek “decent solutions” to challenging constrained optimization problems when standard techniques do not yield optimal results. Such problems are often only tentatively formulated. All candidate solutions we examine, feasible or not, become an innovative database of (biased) samples. Looking beyond merely finding a solution, database queries aid constraint reconsideration, active learning, Pareto frontiers, statistical properties, etc. We also present metrics for comparing populations and tracking their evolutions.

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### CP18 Sensitivity Analysis of Asset Flow Optimization Forecast Algorithm

Asset flow differential equations (AFDE) have been developed and analyzed asymptotically by Caginalp and his collaborators since 1989. We study an inverse problem involving a semi-unconstrained parameter optimization for a dynamical system of nonlinear AFDE from a challenging financial application on investor population dynamics. We present the sensitivity analysis of AFDE and the corresponding asset flow optimization forecast algorithm and the empirical results for a number of closed-end funds trading in US markets.

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### CP18 Set-Valued Measures of Risk

For optimization problems in Mathematical Finance one of the objectives is often to minimize the risk of some financial position. If the investor acts on several markets, under some circumstances risks on different markets can not be aggregated. Then the use of set-valued measures of risk is appropriate. In this paper a complete theory of set-valued risk measures (including primal and dual descriptions) along the lines of the real-valued case is developed. The dual description is based on a new duality theory for set-valued maps, introduced recently by one of the authors.

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### CP18 Risk Optimization Using $p$ -Order Conic Constraints: A Linear Programming Approach

We discuss a class of risk-reward optimization models that reduce to convex programming problems with  $p$ -order conic constraints. As an illustration, a portfolio optimization case study is considered. We develop polyhedral approximation schemes and decomposition algorithms that allow for efficient implementation of the formulated  $p$ -order conic programming models as linear programming problems.

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### CP18 Optimal Portfolio Execution Strategies and Sensitivity to Price Impact Parameters

When liquidating a portfolio of large blocks of risky assets, an institutional investor wants to minimize the cost as well as the risk of execution. An optimal execution strategy minimizes a weighted combination of the expected value and the variance of the execution cost, where the weight is given by a nonnegative risk aversion parameter. The execution cost is determined from a price impact function. Particularly, a linear price impact model is defined by the temporary impact matrix  $H$  and the permanent impact matrix  $\Gamma$ , which represent the expected price depression caused by trading assets at a unit rate. In this paper, we analyze the sensitivity of the optimal execution strategy to estimation errors in the impact matrices under a linear price impact model. We show that, instead of depending on  $H$  and  $\Gamma$  individually, the optimal execution strategy is determined by the combined impact matrix  $\Theta = \frac{1}{\tau}(H + H^T) - \Gamma$ , where  $\tau$  is the time length between consecutive trades. We prove that the minimum expected execution cost strategy

is the naive execution strategy, independent of perturbations, when the permanent impact matrix is symmetric and the combined impact matrix is positive definite. We provide upper bounds on the size of change in the optimal execution strategy in a general setting. These upper bounds are in terms of the changes in the impact matrices, the eigenvalues of a block tridiagonal matrix defined by the combined impact matrix, the risk aversion parameter, and the covariance matrix. These upper bounds indicate that, when the covariance matrix is positive definite, a large risk aversion parameter reduces the sensitivity of the optimal execution strategy. Moreover, when  $\Gamma$  and its perturbation are symmetric, the optimal execution strategy is asymptotically not sensitive to estimation errors when the minimum eigenvalue of either the covariance matrix or the combined impact matrix is large. In addition, our computational results confirm that the sensitivity of the optimal execution strategy to the perturbations decreases, when the permanent impact matrix and its perturbation are symmetric. Moreover, the change in the efficient frontier increases as the risk aversion parameter decreases for asymmetric perturbations. We consistently observe that imposing short selling constraints can reduce the sensitivity of the optimal execution strategy and the efficient frontier.

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#### CP18

##### Quantile-Based Deviation Measures

Quantile-based deviation measures as a class of general deviation measures, defined by Rockafellar et al., have been shown to include all lower semicontinuous law-invariant deviation measures on atomless probability spaces and have been established to be consistent with concave ordering. The latter fact has been used to generalize Rao-Blackwell theorem and to develop an approach for reducing minimization of quantile-based deviation measures to minimization of the measures on subsets of undominated random variables with respect to concave ordering. This approach has been applied for constructing Chebyshev's and Kolmogorov's inequalities with quantile-based deviation measures. As an illustration, Chebyshev's and Kolmogorov's inequalities have been derived for mean absolute deviation, lower semideviation and conditional value-at-risk deviation. Also, an example illustrating advantage of Kolmogorov's inequality with certain deviation measures in estimating the probability in question has been presented.

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#### CP19

##### An Approach for the Robust Optimization of a Biological Objective in Intensity Modulated Radiation Therapy

Intensity Modulated Radiation Therapy (IMRT) is an effective method for delivering precise radiation doses to tumors, while reducing the radiation exposure to surrounding organs-at-risk and normal tissue. We propose a biologically based convex objective function for the utilization in treatment plan optimization models. Given clinically representable criteria, we show that the resulting convex model yields robust treatment plans under possible uncertainties in problem data, and illustrate its use on several test cases.

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#### CP19

##### A Minimal Surface in Molecular Dynamics Simulation of Discoidal High Density Lipoprotein Particles

In a recently concluded work molecular dynamics simulation was used to model the morphology of high density lipoprotein (HDL) particles composed of an apolipoprotein A-1 ring bounding a palmitoylcholine (POPC) bi-lipid membrane under incremental removal of POPC. The study reports the formation of a minimal surface at the interface between two leaflets for one class of HDL particles. We formulate an energy functional for the experiment, consisting of the bending energy of a free ribbon and the surface energy of a membrane and present a gradient descent algorithm for minimizing the functional. The minimal surface obtained as the minimizer of the energy functional with the algorithm is compared to that obtained from the molecular dynamics simulation.

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#### CP19

##### Sequential Methods for Generating Multi-Dimensional Convex Pareto Frontiers

In this presentation, I will discuss a number of new sequential methods for generating multi-dimensional convex Pareto frontiers. Our main motivation for developing these methods is Intensity Modulated Radiation Therapy

(IMRT). All discussed methods are applicable to higher-dimensional problems. Some of the methods can cover the complete Pareto frontier. We also give quality guarantees for the approximation quality of the found Pareto frontier to the real Pareto frontier.

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#### CP19

##### **A Stable Geometric Buildup Algorithm for the Solution of the Distance Geometry Problem Using Least-Squares Approximation**

We propose a geometric buildup algorithm to solve the distance geometry problem in protein modeling, which can prevent accumulation of rounding errors in calculations, tolerate errors in given distances. In this algorithm, we determine each unknown atom by using least-squares approximation instead of exact solution to the system of distance equations. We describe the algorithm, present the test results to determine a set of protein structures with varying degrees of availability and accuracy of distances.

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#### CP19

##### **Clustered Geometric Buildup**

A new method is proposed to solve exact sparse distance geometry problem in 3D space. To avoid numerical error accumulation within incremental geometric buildup algorithm, the following approach is used: a structure is partitioned into overlapping clusters in which the points are computed in no more than a predefined number of incremental buildup generations. The clusters are aligned using least squares method. Results for protein structures with

artificially generated distance data are presented.

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#### CP20

##### **On the Behrens-Fisher Problem: a Globally Convergent Algorithm and a Finite-Sample Study of the Wald, Lr and Lm Tests**

In this paper we provide the first provably convergent algorithm for the multivariate Gaussian Maximum Likelihood version of the Behrens-Fisher problem. Moreover, we establish a systematic algebraic relation between the Wald, Likelihood Ratio and Lagrangian Multiplier Test ( $W \geq LR \geq LM$ ) in the context of the Behrens-Fisher problem. The algorithm allows to computationally investigate the properties of these tests capturing the role of high dimensionality on the actual size and power of the tests for finite samples.

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#### CP20

##### **Construction of Biorthogonal B-Spline Type Wavelet Sequences with Optimal Regularities**

In this paper we study the optimal condition for the refinement coefficients of B-spline type scaling functions such that the corresponding scaling functions are in  $L_2$ . Then the B-spline type wavelet sequences possessing the largest possible regularities and required vanishing moments are characterized, and an optimization algorithm to find such symmetric or antisymmetric B-spline type wavelet sequences is designed.

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#### CP20

##### **Variable Selection via Bridge Regression**

Bridge regression searches a family of  $l_p$  "norm" penalized regressions to choose regression coefficients based on a given model selection criteria. Ridge and lasso regression are special cases of Bridge regression with  $p = 2$  and  $p = 1$ , respectively. Lasso is an effective method for variable selection because it reduces the number of nonzero regression coefficients. When  $0 < p < 1$ , even more coefficients are forced to zero enhancing the variable selection properties of the method. However, when  $0 < p < 1$  the resulting optimization problem is not only non-convex, it



is non-Lipschitzian. In this talk we propose methods for solving these non-Lipschitzian optimization problem. Joint work with James Burke.

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#### CP21

##### **An Object-Oriented Approach to the Implementation of Optimization Algorithms as Abstract Numerical Algorithms**

Many different optimization algorithms can be expressed in a very abstract form just in terms of basic linear operators, vector operations, scalar products, and linear solves. We have coined the term Abstract Numerical Algorithms (ANAs) to describe such algorithms. This presentation will describe the Thyra package and Trilinos object-oriented infrastructure for the development of such algorithms ranging from iterative linear solvers all the way to transient optimization. These algorithms have been implemented independent of the computing model but have been run on production applications on some of our largest parallel machines.

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#### CP21

##### **Preconditioning for Bound Constrained Quadratic Programming Problems**

Recently proposed MPRGP algorithm for the solution of strictly convex quadratic programming problems was proved to enjoy R-linear convergence in bounds on the spectrum. In this talk we consider two methods of preconditioning that improved the theoretical rate of convergence including nonlinear steps, namely preconditioning by a conjugate projector and edge averaging for the variational inequalities discretized by FETI-DP domain decomposition. Theoretical results are confirmed by numerical experiments.

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#### CP21

##### **Optimal Algorithms for Quadratic Programming Problems**

We review our results in development of algorithms for bound and/or equality constrained quadratic programming problems. Their unique feature is the rate of convergence in terms of bounds on the spectrum of the Hessian, independent of representation of the constraints. When applied to the class of convex problems with the spectrum in a given positive interval and sparse Hessians, the algorithms enjoys optimal complexity. The optimality is demonstrated

on the solution of discretized variational inequalities.

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#### CP21

##### **On Convergence of a Rescaled Lagrangian Method To Decompose Structured Convex Programs**

In this paper, we propose a new decomposition method for solving structured optimization problems. The proposed scheme combines the recent decomposition algorithm introduced by Hamdi *et al.* with the nonlinear re-scaling principle of Polyak. The resulting algorithm uses the recently developed non-quadratic multiplier methods based on entropy-like proximal methods, to obtain a family of augmented lagrangian methods which are twice continuously differentiable as opposed to the classical quadratic one. Under mild appropriate assumptions, we show that the method generates convergent primal-dual sequences.

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#### CP21

##### **On Convergence Rate of An Algorithm for Minimizing Quadratic Functions with Separable Convex Constraints**

A new active set algorithm for minimizing quadratic functions with separable convex constraints is proposed by combining the conjugate gradient method with gradient projections. It generalizes recently developed algorithms of quadratic programming constrained by simple bounds. A linear convergence rate in terms of the Hessian spectral condition number is proven. Numerical experiments including frictional 3D contact problems of linear elasticity illustrate the computational performance.

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#### CP22

##### **An Algorithmic Framework for a Class of Non-Convex Minlp Problems**

Solving non-convex Mixed Integer Nonlinear Programming (MINLP) problems with general global-optimization solvers is usually very computationally expensive. To some extent this is related to the decomposition of all functions into elementary ones. We present an algorithmic framework, based on repeated/refined reformulation and approximation, targeted at univariate non-convexity, that works in a geometry that is closer to the original formulation. Computational results are presented.

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**CP22****A Branch-and-Cut Method for Mixed-0-1 Second-Order Cone Programming**

We present a branch-and-cut method for mixed 0-1 second-order cone programming problems. To solve the problems in the nodes of the branch-and-bound tree, we use a primal-dual interior point method, that converges also for infeasible starting points. We use different techniques for the generation of linear and convex quadratic cuts. The quality of the cuts and their impact on the branch-and-bound procedure are investigated. Computational results for test problems and real world applications are given.

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**CP22****Decomposition Strategies for Mixed Discrete Non-Linear Programming**

The proposed paper contributes to the development of the field of Alternating Optimisation for general Mixed Integer Non-Linear Programming (MINLP), by introducing a new decomposition approach based on the Augmented Lagrangian Multipliers method. In the proposed algorithm, the problem has been decomposed to two units, where each set of variables can be optimised by an efficient solver. Particle Swarm Optimization method is used for optimising continuous variables, while a Genetic Algorithm is applied for optimising the discrete variables.

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**CP22****A Method for Optimal Lift Gas Allocation**

An optimal allocation procedure and methodology for the Gas-Lift optimization problem is presented. In the oil industry, natural gas is often injected into the wellbore to assist fluid production in low producing wells and also to compensate sub-surface pressure decline. As the lift gas is constrained and the response to gas injection is non-linear, an optimal allocation is necessary for production maximization. The approach reported is several-fold more efficient than traditional approaches for comparable results.

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**CP22****Computing Safe Dike Heights at Minimal Costs**

Safe dike heights are crucial for protecting life in the Netherlands and many other regions of the world. We

discuss issues that arise when modeling the probability of floods, the expected damage and measures to prevent floods. Our aim is to minimize the sum of future investing costs and expected damage over a long period (of about 300 years). We present some MINLP optimization models and a dynamic programming model, as well as some computational results.

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**CP23****A Trust-region Filter-SQP Method for Mathematical Programs with Linear Complementarity Constraints**

A trust-region filter-SQP method for mathematical programs with linear complementarity constraints (MPLCC) is proposed. We solve a sequence of the relaxed problems with some parameter driven to zero and use the filter technique presented by Fletcher and Leyffer [Math. Program., Ser. A, 91: 239-269 (2002)] to promote the global convergence. Under mild assumptions, it is proved that every accumulation point of the generated iterates is either a strong stationary point or an infeasible stationary point of the MPLCC. Our test problems are originated from the QPECgen generator and include the programs with quadratic and non-quadratic objective functions. Some numerical results are reported, which show that the presented method is very effective.

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**CP23****LPCC Approach to Nonconvex Quadratic Programs**

This talk presents a novel approach to general nonconvex quadratic programs by reformulating them as linear programs with linear complementarity constraints (LPCC). The cornerstone of the approach is a parameter-free min-max integer program formulation of the LPCC, which leads to a finite Benders-type algorithm that involves solving satisfiability subproblems. Computational results are reported on randomly generated problems with two types of constraints: box constraints and general linear constraints, including problems with unbounded feasible regions.

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**CP23****Optimal Control of Elliptic Complementarity Problems in Function Space: C-Stationarity and a Multigrid-Based Solution Scheme**

We consider mathematical programs with complementarity constraints (MPCC) in function space. Typical model problems are related to optimal control of variational inequalities (VIs) or parameter identification in VIs. Based on a smoothed penalization technique C-stationarity is achieved. The proposed algorithm is numerically realized using a semismooth Newton-based full approximation scheme in a multigrid framework. The results are compared to those of an alternative relaxation-method and a report on numerical tests is given.

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**CP23****An  $\ell_1$  Elastic Method for Mathematical Programs with Equilibrium Constraints and Degenerate Programs**

We extend an  $\ell_1$ -elastic framework to the context of MPECs. The resulting smooth equality-constrained subproblems satisfy the MFCQ and are solved using a pre-conditioned interior-point method. Under reasonable assumptions, we establish global convergence to a strongly stationary point provided the penalty parameter remains bounded. We present an implementation of the elastic framework for MPECs and preliminary numerical results. We emphasize how the approach also applies to other types of mathematical programs failing to satisfy the MFCQ.

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**CP23****Structural Topology Optimization Problems Formulated As Mathematical Programs with Equilibrium Constraints**

We consider the technological very important problem of finding minimal weight designs for structural topology optimization problems with *local* stress constraints. The problems are formulated as Mathematical Programs with Vanishing Constraints (MPVC) and as Mathematical Programs with Complementarity Constraints. Some of the theoretical advantages and disadvantages are discussed. We also report several numerical experiments that substantiate the conclusion that MPVCs give a more computational efficient representation for this class of structural topology optimization problems.

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**CP24****Randomized Algorithms for Nonlinear Optimization over Bipartite Matchings and Matroid Intersections**

We consider a broad generalization of the standard linear combinatorial problem which includes a  $d$ -dimensional weight vector for each element and a functional on  $d$ -dimensional space. We compute the objective value applying the functional on the feasible solution weight vector, i.e. the sum of the weight vectors in the corresponding solution. While the problem is generally intractable, we provide randomized algorithms, polynomial for fixed  $d$ , for optimizing arbitrary objectives over bipartite matchings and matroid intersections.

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**CP24****The Graph Embedding and Its Application to QAP**

We introduce a technique for 0-1 integer programming that exploits hypergraph partitioning constraints to produce tight semidefinite program relaxations. We applied the method to quadratic assignment problems and tested on 22 QAP benchmark problems. The method produced SDP bounds within 5% of optimal on average and generated optimal solutions in 10 cases (5 provably optimal). This is the first polynomial time algorithm to achieve provably optimal solutions on any of the benchmark problems.

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**CP24****Path-Based Lp Model of the Set Partitioning Problem**

In this talk, we will present a new, graph-based modeling approach and a polynomial-sized linear programming (LP) formulation of the Set Partitioning Problem (SPP). The approach will be illustrated with a numerical example.

Computational testing and results will be discussed.

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#### CP24

##### The 2-Dimensional Probabilistic Bin Packing Problem

In the probabilistic two-dimensional Bin Packing problem (2D-PBPP), one is asked to pack a random number of rectangular items, without overlap and any rotation, into the minimum number of identical square bins. In this paper we consider the two procedures used for solving probabilistic combinatorial optimization problems: The re-optimization procedure and the a priori one and we focused in their asymptotic behavior through simulations. According to computational results we show that under precise conditions, the best a priori procedure which is a simple method generates results near those given by the re-optimization strategy which is impossible to be carried out.

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#### CP25

##### Optimizing Stability For Polynomial Families

Given a family of polynomials  $\{p\}_x$  whose coefficients depend smoothly on the parameter  $x \in \mathbf{R}^k$ , we seek  $x^*$  to minimize the maximum real part of the roots of the corresponding polynomial  $p_{x^*}$ . This problem is non-smooth, non-convex, and has important applications in stability theory. I consider an approach based on the Routh-Hurwitz conditions, and give some properties of the epigraph of the feasible set.

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#### CP25

##### Variational Analysis of Functions of the Roots of Polynomials

In 2001 Burke and Overton showed that the abscissa mapping on polynomials is subdifferentially regular on the monic polynomials of degree  $n$  in the linear space of polynomials of degree  $n$ . This result is significant for its impact on problems involving optimal stability. In this talk we discuss extensions of this result to a more general class of functions of the roots of polynomials which includes both the abscissa and radius mappings for polynomials.

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#### CP25

##### Advances on the Bessis-Moussa-Villani Trace Conjecture

A long-standing conjecture asserts that the polynomial

$$p(t) = \text{Tr}[(A + tB)^m]$$

has nonnegative coefficients whenever  $m$  is a positive integer and  $A$  and  $B$  are any two  $n \times n$  positive semidefinite Hermitian matrices. The conjecture arises from a question raised by Bessis, Moussa, and Villani (1975) in connection with a problem in theoretical physics. Their conjecture, as shown recently by Lieb and Seiringer, is equivalent to the trace positivity statement above. In this paper, we derive a fundamental set of equations satisfied by  $A$  and  $B$  that minimize or maximize a coefficient of  $p(t)$ . Applied to the Bessis-Moussa-Villani (BMV) conjecture, these equations provide several reductions. In particular, we prove that it is enough to show that (1) it is true for infinitely many  $m$ , (2) a nonzero (matrix) coefficient of  $(A + tB)^m$  always has at least one positive eigenvalue, or (3) the result holds for singular positive semidefinite matrices. Moreover, we prove that if the conjecture is false for some  $m$ , then it is false for all larger  $m$ . Finally, we outline a general program to settle the BMV conjecture that has had some recent success.

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#### CP25

##### Disjunctive Cuts for Non-Convex Mixed Integer Quadratically Constrained Programs

This paper addresses the problem of generating strong convex relaxations of Mixed Integer Quadratically Constrained Quadratic Programs (MIQQP). MIQQP is a very difficult class of problems because it combines two kinds of non-convexities: integer variables and non-convex quadratic constraints. To produce strong relaxations of MIQQP we use techniques from disjunctive programming and lift-and-project. In particular we propose new methods for generating valid inequalities by using the equation  $Y = xx^T$ . We use the concave constraint  $Y - xx^T \succeq 0$  to derive disjunctions of two types. The first ones are directly derived from the eigenvectors of the matrix  $Y - xx^T$  with positive eigenvalues, the second type of disjunctions are obtained by combining several eigenvectors in order to minimize the width of the disjunction. We also use the convex SDP constraint  $Y - xx^T \succeq 0$  to derive convex quadratic cuts and combine both approaches in a cutting plane algorithm. We present series of computational experiments on box-QPs of moderate size.

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#### CP26

##### Scalar Versus Vector Optimization Problems In-

### **olving Risk Functions**

Many risk functions were recently introduced (coherent risk measures, generalized deviations, etc.) and many financial problems were revisited. The use of new risk functions is well justified by the rapid evolution of financial markets and products, but final results often depend on the concrete risk function one draws on. We consider vector optimization problems involving several risk functions and study if the involved objectives may be reduced to a single one capturing every required property.

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### **CP26**

#### **Conic Scalarization in Finite-Dimensional Vector Optimization**

Scalarization approaches to solving vector optimization problems for Pareto optimal points are reviewed and modified for the generation of solutions that are non-dominated with respect to convex cones. The corresponding scalar-valued optimization problems are formulated, classified as linear or nonlinear cone programs, and solved using recent techniques from conic optimization. Based on preliminary computational results, the relevance and implications of using general cones for trade-off or preference modeling in multi-objective programming and decision-making are addressed.

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### **CP26**

#### **Interior Point Warmstarts Applied to Stochastic Programming**

We describe a method of generating a crash-start point for interior point methods in the context of stochastic programming. We construct a small-scale version of the problem corresponding to a reduced event tree and use its solution to generate an advanced starting point for the complete problem. The reduced tree is constructed by scenario aggregation in order to capture information from the scenario space while keeping the dimension of the corresponding (reduced) deterministic equivalent small. Interior point methods struggle in general to take advantage of such information. We derive conditions on the reduced tree that guarantee a successful interior point warm-start for the complete problem. We present numerical results on a range of test problems which shows remarkable advantages of this approach.

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### **CP26**

#### **Multi-Objective Design of a Combinatorial Structure**

A problem of configuring a population of trucks is addressed. The resulting model is a multi-objective optimization problem. We formulate a (single objective) optimization problem to find the best representation of the Pareto optimal set under the constraint that the configurations are built up by common parts. The solution process is also extended to the case when the underlying objective functions are expensive. Results when applying the model to a small industrial example are reported.

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### **CP27**

#### **A Grid-Based Adaptive Simulated Annealing Method for Global Optimization**

A grid-based hybrid method is built that is essentially based on simulated annealing technique. However, this algorithm processes and stores information in several lists as the optimization method tabu does. This technique continuously adjusts the step sizes for different parameters suitably and builds an appropriate annealing schedule in an adaptive manner. The method is implemented on different test functions; comparison centered on accuracy and efficiency is performed with a variant of simulated annealing method.

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### **CP27**

#### **Optimization of Parallel Codes on Cluster of Computers**

Genetic Algorithms are known to be robust and suitable to parallel processing, becoming an attractive approach in the field of numerical optimization. In the research area of aerodynamic optimization, using Computational Fluid Dynamics, the computational efficiency is a major concern. Assuming that a parallel algorithm consists of consecutive stages, a Genetic Algorithm is proposed to find the optimum number of processors and data distribution method to be used for each stage of the parallel algorithm.

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### **CP27**

#### **A New Interval Partitioning approach for Con-**

### strained Optimization

This paper is concerned with solving the continuous Constrained Optimization Problems (COP) with general constraints and objective function. We propose an efficient interval partitioning method (IP) where a new subdivision direction method and an adaptive tree search approach are defined. In the adaptive tree search, nodes are explored using a restricted hybrid depth-first and best-first branching strategy, whereas the new parallel subdivision direction selection rule targets directly the uncertainty degrees of constraints (with respect to feasibility) and the uncertainty degree of the objective function (with respect to optimality). Reducing these uncertainties as such results in the early detection of infeasible and sub-optimal boxes that are discarded reliably. The effectiveness of the proposed IP is illustrated on COP benchmarks and compared with commercial global and local solvers. Key Words: Constrained global optimization, interval partitioning with local search, adaptive search tree management, subdivision direction selection rules

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### CP27

#### A Multistart Approach for Continuous Global Optimization Using a Pseudo-Convexity Criterion

We develop a novel multistart approach for continuous global optimization of expensive functions. In this method, we cluster previously evaluated points such that the data points corresponding to each cluster belong to the graph of a pseudo-convex function. Then, we start a local optimization solver from each cluster. After obtaining new local optimization trajectories, we evaluate additional points in unexplored regions, update the clusters, and then, iterate the procedure. We shall present some numerical results.

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### CP27

#### Low Discrepancy Point Sets Used in Interval Algorithms for Global Optimization

Low discrepancy point sets and low discrepancy sequences are widely used in simulation and estimation algorithms in

science, engineering, finance, industry, and statistical inference. Their application to global optimization is mostly limited to the so-called quasirandom search methods. This talk discusses various usages of them in the framework of interval algorithms for global optimization. Preliminary numerical test results will show what usages are effective and what are not.

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### CP28

#### Sensitivity Analysis for Decentralized Process Control Problems

In this presentation we focus on decentralization of large-scale process control problems. Starting with the Interaction Prediction Principle, we focus on sensitivity issues related to the IPP algorithm and stress that the sensitivity of the overall problem is strongly related to the sub-units. The main result is that different decompositions schemes can lead, under appropriate assumptions, to different sensitivity results for the overall problem.

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### CP28

#### Structured Fixed-Order H-infinity Controller Design

Built upon methods for non-smooth optimization, HIFOO attempts to compute optimal, reduced-order controllers for linear systems. We present extensions to HIFOO allowing the user to input plants with non-trivial feedthrough as well as specify structure on the controller. Finally, HIFOO is applied to try to solve problems in simultaneous stabilization, a known undecidable problem. Numerical experiments are provided for realistic systems, including the control of an industrial web-winding system and structured, static-output-feedback control of an F-16.

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### CP28

#### On Logarithmic Smoothing and Strongly Stable Stationary Points

We consider the problem (P) of minimizing a function over a feasible set  $M$ . By using a logarithmic barrier function, we construct a family  $M^\gamma$  of interior point approximations of  $M$  where  $M^\gamma$  is described by a single smooth inequal-

ity constraint. Under the assumption that all stationary points of (P) are strongly stable we show that there is a one-to-one correspondence between the stationary points of (P) and those of (P $^\gamma$ ) where the latter problem is obtained from (P) by substituting  $M$  by  $M^\gamma$ . Furthermore, corresponding stationary points of (P) and (P $^\gamma$ ) have the same stationary index. The lecture is based on a joint paper with Hubertus Th. Jongen.

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## CP28

### Minimization of Costs in Supply Networks with Transportation and Decision-Making Delays

Due to delays in product transportation and decision-making, supply network dynamics is governed by infinite dimensional differential equations, stability of which is non-trivial to analyze. A unique map revealing stability/instability behavior of the supply network is obtained in the parameter space of the delays, first. Next, an optimization scheme is proposed to choose stabilizing transportation delays that minimize a cost function related to transportation costs and excessive oscillations in inventories. A case study is provided.

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## CP28

### Optimal Grid Synthesis in Control Problems of Prescribed Duration.

Optimal control problems are considered under assumptions that dynamics are nonlinear and running terminal-integral costs are minimized along trajectories on given time intervals. Data are assumed to be Lipschitz continuous relative phase variables. A numerical method is suggested to construct optimal grid synthesis. It is based on a backward procedure of integrating Hamiltonian differential inclusions, and on results of the theory of minimax / viscosity solutions of the Bellman equation. Results of simulations are exposed.

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## CP29

### Design of Electron Devices Using 3D Simulation Codes and Computer Optimization

Computer optimization can explore a larger parameter

space than practical with manual design, particularly for 3D geometries. This allows rapid, economical development of higher performance devices. The proliferation of parametric solid modeling programs allows optimization of both geometry and operating parameters. This presentation will describe computer optimization in the 3D trajectory code Beam Optics Analysis (BOA). In particular, using (BOA) software, we design and model a sheet-beam electron gun, which has the advantage of lower operating voltage, improved efficiency, and greater bandwidth. The physical parameters of the electron gun are then optimized for several different physical goals using parametric modeling software and various sampling based optimization algorithms. Results are presented along with a detailed treatment of the optimization methodology.

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## CP29

### From a Fast Optimization Scheme for the Estimation of Velocity Fields to Image Data Assimilation

We consider the assimilation of satellite images, within the framework of data assimilation in geophysical systems. Based on the constant brightness assumption, we define a nonlinear functional measuring the difference between two consecutive images, the first one being transported to the second one by the unknown velocity. By considering a multiscale approach and a Gauss-Newton minimization algorithm, we can estimate the entire velocity fields at a high frame rate and then assimilate these pseudo-observations.

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## CP29

### Convex Iteration for Constraining Cardinality and Rank with Application to Compressive Sampling

We present a numerical technique, called convex iteration, originally conceived for constraining rank in semidefinite programming. The technique possesses an analog for constraining cardinality. Recent results from compressed sensing (a.k.a, compressive sampling) theory establish cardinality as a lower bound on number of measurements required to obtain perfect reconstruction. We present examples, from signal processing and particularly Magnetic Resonance Imaging (MRI), achieving that lower bound while retaining perfect reconstruction. We demonstrate robustness of the algorithm in presence of noise.

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**CP29****Nonnegative Matrix Factorization and Underapproximation**

Nonnegative Matrix Factorization (NMF) is a compression technique which allows interpretation of nonnegative data, with applications in image processing, text mining, etc. We study an extension called Nonnegative Factorization (NF) consisting in finding the best approximation of a not-necessarily nonnegative matrix by a product of two low-rank nonnegative matrices and use it within a new underapproximation technique (NMU) particularly efficient at achieving sparse solutions for NMF. We also show NP-hardness of both (NF) and (NMU).

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**CP29****Optimization Methods for Improving Video Field of View**

The field of view of modern digital video cameras can be significantly increased by optically superimposing different regions of a scene and then computationally disambiguating the superimposed frames. The aim of this process is to generate a high resolution, wide field of view video without a large and potentially expensive detector array. In this talk, we present computational methods for solving the disambiguation problem associated with such a system. Building upon existing optimization methods for solving the  $\ell^2 - \ell^1$  minimization problem associated with static compressed sensing, we develop a fast approach designed to exploit the dynamics of the video setting. Simulation and experimental results demonstrate the effectiveness of this approach over non-dynamic approaches.

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**CP30****Resource-Constrained Scheduling in Computer Games**

This paper studies a resource-constrained project scheduling problem. Consider a set of tasks each of which is associated with three parameters: the amount of required resources, the amount of returned resources and the processing time. Given an initial resource level, we want to determine a feasible mission sequence such that we can meet the target resource level in the earliest time. In this paper, we design and analyze several approximation algorithms.

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**CP30****Design of Fixed-Order Robust Controllers via Non-smooth Optimization**

HIFOO (H-infinity fixed-order optimization) is a MATLAB package for fixed-order controller design using nonsmooth, nonconvex optimization. We discuss the practical application of HIFOO to solve real-world problems from the engineering literature. We also introduce a new version of HIFOO that is designed to find controllers that, in addition to achieving good performance and robustness, are also strongly stable. Benchmarks on real-world problems are presented.

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**CP30****Hybrid Optimization Techniques for Hydrodynamic Stability Control**

We propose a numerical scheme for the solution of problems of hydrodynamic stability control. In that context we consider shape optimization problems in flow control where the stability issues are represented by eigenvalue constraints. We investigate approaches based on a combination of derivative-free and gradient-based methods with focus on an adequate treatment of the eigenvalue function. Moreover, techniques relying on high-performance computing are used to solve the resulting large highly nonlinear systems.

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**CP30****Convex Conic Formulation of Upper Bound Element Techniques in Metal Forging**

The upper bound element technique (UBET) is an alternative to finite element methods for engineering problems in applied plasticity. UBET requires solving sequences of non-smooth optimization problems that reflect the dynamic geometry of the workpiece and the need to evaluate competing manufacturing designs. We show that, in the context of metal forging, UBET problems can be reformulated in terms of sparse convex conic optimization. We also present



some preliminary computational results.

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### MS1

#### **Nonsmooth Algorithms for Nonlinear Semidefinite Programming**

Applications to automatic control have been among the driving forces to develop methods for nonlinear semidefinite programming (NL-SDP). For instance, the Kalman-Yakubovic-Popov Lemma leads to programs subject to bilinear matrix inequality (BMI) constraints. These BMIs are hard to solve due to a strong disparity between the unknown controller gains and the Lyapunov variables. For sizeable systems, the best results are to date obtained by nonsmooth optimization methods [1]. For H infinity synthesis a new line was proposed in [2], where the use of Lyapunov variables can be avoided. In this presentation we develop these ideas further and address several interesting applications, like parametric robustness [3] or mixed (multi-objective) control [4]. [1] P. Apkarian, D. Noll, O. Prot. A trust region spectral bundle method for nonconvex eigenvalue optimization. 2007. [2] P. Apkarian, D. Noll. Nonsmooth H infinity control. IEEE Trans. Autom. Control. 51, no. 1, 2006, 71-86. [3] P. Apkarian, D. Noll, O. Prot. Nonsmooth methods for control design with IQCs. 2007. [4] P. Apkarian, D. Noll, A. Rondepierre. Mixed H2/H infinity control via nonsmooth optimization. 2007.

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### MS1

#### **A New First Order Method for Non-Linear Semidefinite Programming**

A new method for the efficient solution of nonlinear optimization problems with matrix variables is introduced. The method is based on the sequential convex programming concept. The main idea is to approximate nonlinear functions defined in matrix variables by sequences of block separable, convex functions. The resulting subproblems are convex semidefinite programs with a favorable structure, which can be efficiently solved by the code PENNON. Convergence results as well as numerical experiments are presented. Finally it is shown how the method can be generalized for the solution of standard nonlinear semidefinite programs.

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### MS1

#### **A Derivative Free Method for Nonlinear SDPs**

At the moment, most available algorithms for SDPs aim at the efficient solution of (high dimensional) linear, maybe even nonlinear, problems. Most methods therefore rely on first or even second-order information. In contrast to this, we will focus on a completely derivative-free method for nonlinear SDPs. We will highlight both theoretical and practical aspects of the algorithm, which actually is the derivative-free version of the penalty-barrier-multiplier method used for example in pennon.

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### MS1

#### **Primal-Dual Interior Point Methods for Nonlinear SDP Problem**

In this talk, a class of primal-dual interior point methods for nonlinear SDP problems will be presented. It will be shown that globally convergent primal-dual algorithms which are similar to methods for usual nonconvex NLP problems can be developed for nonconvex NLSDP problems. Various possibilities for search strategy including line search and trust region methods, for merit function selection including primal function and primal-dual function, along with our numerical experiment will be presented.

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### MS2

#### **A Class of Inexact Null Space Iterations in PDE-Constrained Optimization**

Based on linearly convergent iterative solvers for the state and the adjoint equation, respectively, a preconditioned iterative scheme for the KKT-system of class of discretized PDE-constrained minimization problems is proposed. Every step of the outer loop may be interpreted as a SQP-type step. The inner loop consists essentially of two parts: approximate feasibility restoration and a step towards optimality. The globalization is based on a  $\ell_1$  line search. A convergence analysis of the method is provided and numerical results are presented.

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### MS2

#### **An Adjoint Approach to Shape Optimization in Computational Fluid Dynamics**

We consider shape optimization problems governed by the stationary incompressible Navier-Stokes equations. In contrast to fully discrete methods the shape derivatives are computed analytically by using a continuous adjoint-based

approach. For the stationary problem we use pseudo-time marching in connection with preconditioning and suitable time stepping schemes that can be applied in parallel for the state and adjoint equation. Numerical results will be presented.

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## MS2

### Numerical results with a Multilevel Trust-Region Method in Infinity Norm

We present a multilevel trust-region method in infinity norm for both unconstrained and bound constrained optimization. The main feature of the new method is to allow the exploitation, in a trust-region framework, of the fact that many large-scale optimization problems have a hierarchy of different descriptions, possibly involving different number of variables. The important features and parameters of the algorithm are described. Extensive numerical results are presented on a set of problem arising in PDE based optimization. The general behaviour of the algorithm is analysed first as a function of its parameters. Comparison with other optimization algorithms is also provided.

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## MS2

### A Posteriori Error Estimators Based on Weighted KKT-Residuals for Adaptive Control Constrained

## Optimization with PDEs

We introduce a concept for reliable a posteriori error estimators for a class of control constrained optimization problems with PDEs (including elliptic or parabolic problems). We show that an appropriate weighted residual (in function space) of the KKT-conditions, which is motivated by interior point methods, yields a reliable error estimator for approximate solutions of the optimality system. For finite element discretizations this residual can be estimated elementwise by using standard error estimators, which results in a reliable error estimator for adaptive mesh refinement. Numerical results are presented.

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## MS3

### Error Estimates in the Approximation of Optimal Control Problems Governed by Quasilinear Elliptic Equations

In this talk we consider an optimal control problem governed by the quasi-linear elliptic equation

$$-\operatorname{div}[a(x, y(x)) \nabla y(x)] + f(x, y(x)) = u(x) \text{ in } \Omega, \quad (1)$$

$$y(x) = 0 \text{ on } \Gamma \quad (2)$$

where  $a(x, y) \geq \alpha > 0$  and  $f$  is monotone non-decreasing with respect to the second variable. The goal is to carry out the numerical analysis of the control problem providing some error estimates of the approximations. Though the state equation is well posed, the uniqueness of a solution of the discrete state equation is an open problem. In the analysis the following steps are performed:

- The discrete state equations are locally well posed and we obtain error estimates for the approximations.
- We prove that strict local minima of the control problem can be approximated by local minima of the discrete problems.
- By assuming that a local minimum satisfies the sufficient second order optimality condition, we get error estimates for the discrete approximations.

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## MS3

### A Moreau-Yosida Based Regularization Scheme for Pointwise State Constraints in PDE-Constrained Optimization

The generalized Moreau-Yosida regularization of the characteristic function of several classes of pointwise state constraints in optimal control of PDEs is considered. Its flexibility allows to treat different constraint types (such as distributed or boundary constraints) within one unifying framework. Under a mild assumption we derive existence of Lagrange multipliers as well as the convergence of the

regularization scheme. A function space based solution method is introduced and its convergence is analysed. The talk ends by a report on numerical tests.

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### MS3

#### **Neuman and Dirichlet Boundary Control - Optimal Convergence Rates and Numerical Implementation**

We discuss tailored discretization concepts for elliptic Neumann and Dirichlet boundary control problems and prove optimal error bounds on the control variables. We present numerical examples which confirm our analytical findings.

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### MS3

#### **The Goal Oriented Dual Weighted Approach for Control and State Constrained Elliptic Optimal Control Problems**

We consider primal-dual weighted goal oriented a posteriori error estimates for pointwise control and state constrained optimal control problems associated with second order elliptic partial differential equations. The estimators are derived within the framework of the goal oriented dual weighted approach. They consist of primal-dual residuals, primal-dual weighted error terms representing the mismatch in the complementarity system due to discretization, and data oscillations. In case of sufficiently regular active (or coincidence) sets and problem data, a further decomposition of the multiplier into a regular  $L^2$ -part on the active set and a singular part concentrated on the boundary between active and inactive set allows a further characterization of the mismatch error. Numerical results are given to illustrate the performance of the error estimators.

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### MS4

#### **An Outer-Approximation Approach to Maximum Entropy Sampling with Quadratic Constraints**

This work presents an outer-approximation algorithm for maximum entropy sampling with quadratic constraints. A new mixed-integer semidefinite program formulation that employs binary variables to indicate the selection of a sampling point, and exploits the linear equivalent form of a bilinear term involving binary variables to ensure convexity. An outer-approximation algorithm that obtains the optimal solution by solving a sequence of mixed-integer linear programs is developed. Numerical experiments verify the

computational effectiveness of the proposed method.

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### MS4

#### **Pump-Based Heuristics for Mixed-Integer Nonlinear Programming**

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### MS4

#### **A Lifted Linear Programming Branch-and-Bound Algorithm for Mixed Integer Conic Quadratic Programs**

We develop a linear programming based branch-and-bound algorithm for mixed integer conic quadratic programs, which is based on a higher dimensional or lifted polyhedral relaxation of conic quadratic constraints introduced by Ben-Tal and Nemirovski. We present results of computational experiments on a series of portfolio optimization problems and show that the algorithm significantly outperforms commercial and open source solvers based on both linear and nonlinear relaxations.

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### MS5

#### **Polynomial Optimization Techniques for Second Order PDEs and Optimal Control Problems**

To solve a partial differential equation (PDE) numerically, we formulate it as a polynomial optimization problem (POP) by discretizing it via a finite difference approximation. The resulting POP satisfies a structured sparsity, which we exploit by applying the sparse SDP relaxation of Waki et al. to obtain an approximate solution of the PDE. Moreover, we take into account the particular structure of POP's feasible set, determined by equality constraints, to reduce the size of the sparse SDP relaxation.

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### MS5

#### Semidefinite (SDP) Representation of Convex Sets

A set  $S \subset R^n$  is called SDP representable if  $S$  equals the projection of a set in  $R^{n+N}$  describable by some LMI. Clearly, the necessary conditions are  $S$  must be convex and semialgebraic. This talk discusses sufficient conditions and necessary conditions for SDP representability. We will prove: **(1)** Suppose  $S = \{x : g_1(x) \geq 0, \dots, g_m(x) \geq 0\}$  is a compact convex set defined by polynomials. Then  $S$  is SDP representable if each  $g_i(x)$  is sos-concave, i.e.,  $-\nabla^2 g_i(x) = W(x)^T W(x)$  for some possibly nonsquare matrix polynomial  $W(x)$ . **(2)** For a general compact convex semialgebraic set  $S$ , we prove the sufficient condition: the boundary of  $S$  is positively curved, and the necessary condition: the boundary of  $S$  has nonnegative curvature at smooth points and on nondegenerate corners. A sufficient condition bypassing the gaps is when some defining polynomials are sos-concave.

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### MS5

#### Optimization with Polynomials

Optimization problems involving multivariate polynomials are ubiquitous in many areas of engineering and applied mathematics. Although these problems can sometimes (but not always) be approached using the traditional ideas of nonlinear optimization, in recent years there has been much interest in new techniques, that exploit their intrinsic algebraic features, to provide global solutions and/or more efficient algorithms. In this talk we survey the basic features of these algebraic approaches, involving sum of squares (SOS) and semidefinite programming, emphasizing the geometric aspects and a few selected applications in dynamical systems and game theory.

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### MS5

#### Perfect Point Configurations

We study a problem of Lovasz as to when a real point configuration has the property that all linear polynomials that are non-negative over the points are also sums of squares of linear polynomials modulo a radical zero-dimensional ideal whose variety has exactly these given points as the real points in it. This leads to a generalization of Lovasz's theta body for a graph to all polytopes which is a semidefinite

relaxation of the polytope.

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### MS6

#### A Variant of the Augmented Lagrangian Method with Faster Dual Convergence

In this talk we discuss a variant of the augmented Lagrangian method in which a different update rule is used to generate the sequence of dual Lagrange multipliers. Arithmetic-complexity results are derived for two stopping rules in the context of a special but broad class of convex programs. Specializations of these results are also derived in the context of the cone programming problem.

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### MS6

#### A Primal-Dual First-Order Method for Linear Cone Programming

We first reformulate a linear cone programming into a primal-dual smooth convex minimization problem over a manifold. Then we discuss Nesterov's smooth method for solving them, and the associated iteration-complexity bound is discussed. The proposed method is finally applied to solve some large-scale linear cone programming problems arising from compressed sensing. The computational results show that this method substantially outperforms interior point methods, and is very promising to solve this class of large-scale problems.

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### MS6

#### Arithmetic-Complexity of Augmented Lagrangian Algorithms.

In this talk, we discuss arithmetic-complexity results for a classical optimization algorithm, namely: the augmented Lagrangian method, in the context of a special but broad class of convex programs. In particular, we present specialization of these complexity results in the context of the conic programming problem.

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### MS6

#### An ACCPM Algorithm for Support Vector Ma-

**chine Classification with Indefinite Kernels.**

In this paper, we propose a method for support vector machine classification using indefinite kernels. Instead of directly minimizing or stabilizing a nonconvex loss function, our method simultaneously finds the support vectors and a proxy kernel matrix used in computing the loss. This can be interpreted as a robust classification problem where the indefinite kernel matrix is treated as a noisy observation of the true positive semidefinite kernel. Our formulation keeps the problem convex and relatively large problems can be solved efficiently using the analytic center cutting plane method. We compare the performance of our technique with other methods on several data sets.

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**MS7****Title TBD**

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**MS7****Title TBD**

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**MS8****Robust Optimization to the Rescue of Chance Constraints**

We study conic optimization problems affected by stochastic uncertainty under partial information on the underlying probability distribution functions. In the Chance Constraints (CC) approach feasibility is required to hold with at least a given probability. Such problems are notoriously difficult. We show that the Robust Optimization methodology can offer safe and tractable approximations to these CC problems.

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**MS8****Robust Discrete Optimization**

Abstract not available at time of publication.

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**MS8****Less is More: Robustness and Sparsity in Multivariate Statistics**

We describe applications of robust optimization in the context of machine learning, with a focus on classification and regression, principal component analysis and fitting of graphical models. In these tasks, sparsity of the solution is often desired as it provides ways to interpret the result. In a classification problem for example, the sparsity pattern of the classifier vector allows to identify the features that are most discriminative. We will explore the connections between sparsity and robustness and illustrate these connections in the context of genomic data, as well as social data, such as voting records and online news.

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**MS8****Robust Optimization in Multi-Period Problems**

We discuss computational tractability of Affinely Adjustable Robust Counterpart of an uncertain Linear Programming problem, with emphasis on a generic application, specifically, on computationally efficient design of affine control rules for an uncertainty-affected linear dynamical system ensuring that the state-control trajectory on a given finite horizon satisfies in a robust fashion a system of linear inequalities.

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**MS9****Active-Set Approaches to Basis Pursuit Denoising**

Many imaging and compressed sensing applications seek sparse solutions to large under-determined least-squares problems. The basis pursuit (BP) approach minimizes the 1-norm of the solution, and the BP denoising (BPDN) approach balances it against the least-squares fit. The duals of the BP and BPDN problems are conventional linear and quadratic programs. We explore the effectiveness of active-set approaches for solving large-scale BP and BPDN problems.

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**MS9****Iterative Signal Recovery From Incomplete and Inaccurate Measurements**

Compressive Sampling (CoSa) offers a new paradigm for acquiring signals that are compressible with respect to an orthobasis. The major algorithmic challenge in CoSa is to approximate a compressible signal from noisy samples.

Until recently, all provably correct reconstruction techniques have relied on large-scale optimization, which tends to be computationally burdensome. This talk describes a new iterative, greedy recovery algorithm, called CoSaMP that delivers the same guarantees as the best optimization-based approaches. Moreover, this algorithm offers rigorous bounds on computational cost and storage. It is likely to be extremely efficient for practical problems because it requires only matrix-vector multiplies with the sampling matrix. For many cases of interest, the running time is just  $O(N * \log^p(N))$ , where  $N$  is the length of the signal and  $p$  is a small integer.

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## MS9

### Sparse Reconstruction via Separable Approximation

Finding sparse approximate solutions to large underdetermined linear systems of equations is a common problem in signal/image processing and statistics. One standard approach is to minimize the sum of a quadratic error term and a sparsity-inducing (usually  $\ell_1$ ) regularization term. We propose iterative methods in which each step is obtained from an optimization subproblem involving a separable quadratic term plus the original sparsity-inducing term. Our approach handles group-separable regularizers in addition to the standard  $\ell_1$  regularizer.

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## MS9

### First-Order Methods for Constrained and Unconstrained $\ell_1$ -Minimization Problems

We propose simple and efficient methods for solving the problems  $\min_u \mu \|u\|_1 + \|Au - f\|^2/2$  and  $\min_u \{\|u\|_1 : Au = f\}$ , respectively, which are used in compressed sensing. Our method for the unconstrained problem is based on operator splitting and continuation. We show that this method obtains the support and signs of the optimal solution in a finite number steps, and achieves a  $q$ -linear global

convergence speed. Our method for the constrained problem is based on Bregman iterative regularization and yields an exact solution after solving only a very small number of instances of the unconstrained problem above for  $f = f^k$  given. We show analytically that this iterative approach is equivalent to the method of multipliers. Both methods are especially useful for many compressed sensing applications where matrix-vector operations involving  $A$  and  $A'$  can be computed by fast transforms. We were able to solve huge instances of compressed sensing problems quickly on a standard PC.

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## MS10

### Optimizing the Probe Placement for Radio-Frequency Ablation

The focus of this talk will be on the RF ablation of liver tumors with mono- or bipolar systems. To achieve a complete destruction of the lesion, one has to consider a number of various effects as for example the cooling influence of blood vessels and the patient individual tissue properties. In this talk different approaches towards an optimization of the RF probe placement (as e.g. an optimization with an analytic approximation of the electric potential, a multi-scale optimization, and a stochastic optimization taking the uncertainty in the tissue parameters into account) will be discussed. Moreover, applications of the optimization to artificial test scenarios as well as to a real RF ablation will be presented.

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## MS10

### Identification of Tissue Properties for Thermal Ablation

We focus on the identification of thermal and electrical

conductivities for thermal ablation, e.g. radio-frequency ablation. From measurement data of the temperature distribution the parameters are reconstructed by formulating the inverse problem as an optimal control problem. Thus, we solve a minimization problem with the heat equation and the potential equation as constraints, and where those two equations are coupled through source terms of the heat equation. We use a finite element method to solve the constraining PDE system. Various examples demonstrate the performance of our approach.

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### MS10

#### Identification of Perfusion and Antenna Profiles in Regional Hyperthermia

In the cancer therapy regional hyperthermia, the most prominent modeling errors stem from the highly individual perfusion arising in the bio-heat transfer equation. The talks presents identification of the perfusion based on MR thermography data, aiming at both, quality assessment and online reoptimization. A second area affected by several sources of model errors is the computation of specific absorption rates. A possibility to improve the SAR model again using MR thermography will be discussed.

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### MS11

#### A Fast Method for Finding the Global Solution of the Regularized Structured Total Least Squares Problem for Image Deblurring

Given a linear system  $Ax \approx b$  where both the structured matrix  $A$  and the vector  $b$  are subject to noise, the structured total least squares (STLS) problem seeks to find a correction matrix and a correction righthand side vector of minimal norm which makes the linear system feasible while maintaining the structure of  $A$ . To avoid ill-posedness, a regularization term is added to the objective function; this leads to the so-called regularized STLS (RSTLS) problem. In general this problem is nonconvex and hence difficult to solve. However, we show that problem can be globally and efficiently solved for structures arising from image deblurring applications under reflexive or periodic boundary conditions. The devised method is based on decomposing the problem into single variable problems and then transforming them into 1D unimodal real-valued minimization problems which can be globally solved. Based on uniqueness and attainment properties of the RSTLS solution we show that a constrained version of the problem possess a strong duality result and can thus be solved via a sequence of RSTLS problems.

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### MS11

#### Augmented Primal-Dual Method for Linear Conic Programs

We propose a new iterative approach for solving linear programs over convex cones. Assuming that Slater's condition is satisfied, the conic problem is transformed to the minimization of a certain convex differentiable function. The evaluation of the function and its derivative is cheap if the projection of a given point onto the cone can be computed cheaply, and if the projection of a given point onto the affine subspace defining the primal problem can be computed cheaply. For the special case of a semidefinite program, a certain regularization of this function is analyzed. Numerical examples illustrate the potential of the approach.

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### MS11

#### Robust Limit Analysis of Steel Structures

We study the problem of limit analysis of elastic structures, i.e., problem of finding the maximal multiplier of a given load, such that the new load can still be supported by the structure. This is measured by the von Mises failure criterion. The problem can be formulated as an SOCP. We will assume that the loads are not exact, rather perturbed by small perturbation loads lying in an ellipsoid. The robust counterpart to our SOCP is then a linear SDP. We will compare solutions of this SDP with solutions of approximate robust counterparts due to Bertsimas and Sim and to Goldfarb and Iyengar. We will show that, for this particular problem, the exact robust counterpart is far superior to the approximate ones. We will further show that the so-called shake-down analysis due to G. Maier is a special approximate robust counterpart of the standard limit analysis problem.

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### MS11

#### Matrix Convex Functions and Optimization

In this talk, we discuss various differentiation rules for general smooth matrix-valued functions, and for the class of matrix convex (or concave) functions first introduced by Löwner and Kraus in the 1930s. For a matrix monotone function, we present formulas for its derivatives of any order in an integral form. Moreover, for a general smooth primary matrix function, we derive a formula for all of its derivatives by means of the divided differences of the original function. As applications, we use these differentiation rules and the matrix concave function  $\log X$  to study a new notion of weighted centers for Semidefinite Programming (SDP). We show that, with this definition, some known properties of weighted centers for linear programming can be extended to SDP. We also show how the derivative formulas can be used in the implementation of barrier methods for optimization problems involving nonlinear but convex matrix functions. This talk is based on a joint paper with Jan Brinkhuis and Tom Luo.

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### MS12

#### A Multilevel Algorithm for Inverse Problems with Elliptic PDE Constraints

We propose a multilevel algorithm for the solution Tikhonov-regularized first-kind Fredholm equations. We consider a source identification problem in which the forward problem is an elliptic partial differential equation. Our method assumes the availability of an approximate Hessian operator for which, first, the spectral decomposition is known, and second, there exists a fast algorithm that can perform the spectral transform. Based on this decomposition we propose a Conjugate Gradients solver which we precondition with a multilevel subspace projection scheme. We demonstrate the effectiveness of our method with the 2D-Neumann Poisson problem with variable coefficients and partial observations.

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### MS12

#### Shape Optimization Governed by the Linear Elasticity Equations

Using sheet metal forming a wide variety of different profiles can be manufactured. We apply shape optimization to help find the optimal design for a given application. We present an efficient multilevel SQP-method for the non-convex geometry optimization of sheet metal profiles, which is also suited for other design problems. We use detailed PDE-based models, e.g., 3D linear elasticity for stiffness optimization, which is the focus of this talk, or

the heat equation. Numerical results are presented.

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### MS12

#### Numerical Methods for Experimental Design of Ill-Posed Problems

In this talk we present a method for the design of experiments in the context of parameter identification problems. We develop a new methodology based on empirical risk minimization, that enable us to use modern PDE optimization methods for the design of such experiments.

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### MS12

#### Computing Hessian Approximations for Partially Separable Unconstrained Optimization

In Newton-like methods, computing Hessian, or some dense approximation, represents a serious obstacle to solve large-scale unconstrained optimization problems because of the still limited computation resources and memory capacities. Fortunately, these problems often have a partially separable structure. We present and compare several ways to approximate Hessian taking advantage of this property without requiring more than function and gradient evaluations. Some numerical experiences inside a recursive multilevel trust-region algorithm are also presented. A better integration in this framework is currently under investigation by trying to use information from approximate invariant subspaces and multisection equations.

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### MS13

#### Interface Evolution: A Control Problem with $H^1$ - and $H^{-1}$ -Norms in the Cost Functional

Interface evolution with mass conservation can be modelled by the Cahn-Hilliard equation, which is a variational inequality of fourth order. Discretizing in time the corresponding gradient flow equation results into a control problem with control constraints and with a cost functional including the  $H^1$ -semi-norm as well as the norm of the dual space  $H^{-1}$ . Hence, we face problems similar to control problems with state constraints. First we present shortly the existence results for the control. As main focus of this talk we discuss the application of the primal-dual active set method, analyse its convergence behaviour and present numerical results. One further aspect is the efficient solution of the resulting linear systems having saddle point structure. This freedom of choosing a linear algebra solver



is one advantages of using the primal-dual method instead of other simulation approaches. A further advantage is the enormous reduction of the dimension due to small inactive sets. A short outlook on interface evolution without mass conservation with the Allen-Cahn variational inequality is given at the end.

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### MS13

#### Structure Exploiting A-Priori and A-Posteriori Discretization Concepts for Elliptic Optimal Control Problems in the Presence of Gradient Constraints

We consider optimal control problems subject to an elliptic (possibly nonlinear) partial differential equation with constraints on the gradient of the state. We introduce a tailored appropriate discretization concept. The state equation is discretized with the help of lowest order Raviart Thomas mixed finite elements to cope with possible discontinuities for the control and the adjoint state. In order to solve the discretized problems efficiently structure exploiting numerical solution algorithms are discussed. Furthermore optimal error estimates for the numerical finite element solution are presented. In the context of goal-oriented adaptivity the DWR concept proposed by Becker and Rannacher for PDE-constrained optimization is extended to our framework. With the help of an error representation in the objective local error indicators are defined. Their performance properties are investigated by means of numerical examples.

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### MS13

#### Balancing Regularization and Discretization Error in the Virtual Control Concept for State-Constrained Optimal Control Problems with Boundary Control

We consider a linear quadratic optimal control problem with pointwise state constraints and control constraints, where the control acts at the boundary. It is well known that problems with pointwise state constraints inhibit a lot of difficulties since the Lagrange multipliers are in general only Borel measures. Therefore, different regularization concepts are developed in the last years. However, a direct extension of the Lavrentiev regularization concept is not possible since the control is not defined in the domain where the state constraints are given. We will use the concept of a virtual distributed control in the domain  $\Omega$ . Thus the Lavrentiev regularization is applicable. The effect of regularization is influenced by different parameter functions depending on a regularization parameter  $\varepsilon > 0$ .

Furthermore, the problem is discretized by finite elements. We derive an error estimate of the optimal solution of the original problem to the corresponding discretized and regularized one. Since the regularization error and the discretization error appears simultaneously, we have to balance the regularization parameter and the mesh size in an appropriate manner.

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### MS13

#### Feedback Stabilization of the Navier-Stokes Equations by a Boundary Control of Finite Dimension

We are interested in the stabilization of the Navier-Stokes equations in a neighbourhood of an unstable stationary solution. When the Reynolds number becomes large enough the discretization of the equations requires a high number of degree of freedom. In that case the numerical solution of the Riccati equation needed to define a feedback control cannot be calculated. In this talk we shall show that a control of finite dimension is sufficient to stabilize (locally) the full nonlinear equation. This kind of result has been already obtained in the case of a distributed control, but in our knowledge is new in the case of a boundary control.

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### MS14

#### Acyclic and Star Coloring Algorithms for Hessian Computation

The following four-step procedure makes the computation of a sparse Hessian  $H$  using automatic differentiation efficient: determine the sparsity pattern of  $H$ ; using an appropriate graph coloring, obtain a seed matrix  $S$ ; compute the compressed Hessian  $B \equiv HS$ ; recover the values of the entries of  $H$  from  $B$ . We discuss novel algorithms developed within CSCAPES for each of these steps, with emphasis on the coloring step. We also sketch a framework for parallelizing greedy coloring algorithms.

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### MS14

#### Pattern Graphs for Sparse Matrices

Abstract not available at time of publication.

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**MS14****Coloring Hierarchical Derivative Matrices**

Discretizing PDEs on a regular grid induces a hierarchy of two types of sparsity patterns on a Jacobian matrix, one due to the stencil being used and one due to the dependence among individual degrees of freedom within that stencil. Goldfarb and Toint demonstrated how to exploit the sparsity structure induced by the stencil, but exploiting the unstructured sparsity within the stencil must rely upon more general techniques. We present a two stage coloring strategy: Goldfarb-Toint coloring followed by optimal intra-stencil coloring. We demonstrate that optimal coloring at both stages is suboptimal in general. Nonetheless, savings of 50% or more over Goldfarb-Toint alone are possible.

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**MS14****Sparsity Detection for Jacobians and Hessians in ADOL-C**

Abstract not available at time of publication.

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**MS15****Overview of the Minisymposium, and Recent Results on the Application of Semidefinite Programming to Characterize Satisfiability**

This presentation will first provide a brief overview of the minisymposium. Second, a new semidefinite programming relaxation for the satisfiability problem will be presented. This relaxation is an extension of previous relaxations arising from the paradigm of partial semidefinite liftings for 0/1 optimization problems. It is shown that the relaxation is exact for Tseitin instances with no restrictions on their structure, meaning that the instance is unsatisfiable if and only if the corresponding semidefinite relaxation is infeasible.

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**MS15****Solving Minimum  $k$ -Partition Problems Using Semidefinite Programming**

The minimum  $k$ -partition ( $MkP$ ) problem is the problem of partitioning the set of vertices of a graph into  $k$  disjoint subsets so as to minimize the total weight of the edges joining vertices in the same partition. Our main contribution is the design and implementation of a branch-and-cut algorithm based on semidefinite programming (SBC) for the  $MkP$  problem. The two key ingredients for this algorithm are: the combination of semidefinite programming with polyhedral results; and a novel iterative clustering heuristic (ICH) that finds feasible solutions for the  $MkP$  problem. The SBC algorithm computes globally optimal

solutions for dense graphs with up to 60 vertices, for grid graphs with up to 100 vertices, and for different values of  $k$ , providing the best exact approach to date for  $k \geq 3$ .

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**MS15****Solving Quadratic 0-1 and Max-Cut Problems by Semidefinite Programming**

In this talk we present a method for finding exact solutions of the Max-Cut problem (MC), an NP-hard combinatorial optimization problem. This method is based on a relaxation of MC using Semidefinite Programming (SDP) combined with a polyhedral relaxation by incorporating the so-called triangle inequalities. We use a branch and bound framework, applying this relaxation as upper bound. The computation of this upper bound is done by a dynamic version of the bundle method. This algorithm has been introduced as Biq Mac - a solver for Binary Quadratic and Max-Cut problems. Besides explaining in detail the algorithm, we also present many numerical results, collected as Biq Mac Library. Furthermore, we review other solution approaches and compare the numerical results with our method. The experiments show, that our method nearly always outperforms all other approaches. In particular, where Linear Programming based methods fail (i.e. dense graphs) our method performs very well. Exact solutions are obtained in reasonable time for any instance of size up to  $n=100$  vertices, no matter what density. Various test problems that have been considered in the literature for years, were solved by Biq Mac for the first time.

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**MS15****Local Branching with Semidefinite Relaxations**

We investigate the application of semidefinite relaxations to the Local Branching scheme that was recently introduced for integer programming problems. Our motivation is two-fold: First, we aim to improve the Local Branching framework through higher-quality starting solutions and stronger relaxations. Second, we aim to develop search

heuristics to efficiently apply semidefinite relaxations to combinatorial problems. We demonstrate our findings experimentally on different problem domains, including stable set and max-2sat problems.

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### MS16

#### ***T*-Algebras and Linear Optimization Over Symmetric Cones**

The first target-following algorithm was given by Shinji Mizuno in 1992 for linear complementarity problems, using the notion of delta sequences. The delta sequence is a sequence of targets that lead the primal-dual solutions towards optimality. This target-following paradigm was successfully generalized to semidefinite programming by the speaker in a recent work. In this talk, the target-following framework is further generalized to symmetric cone programming via *T*-algebra.

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### MS16

#### **Invariance Properties of Extremal Ellipsoids of a Convex Body**

Let  $K$  be a convex body in a finite dimensional Euclidean space. The minimum volume ellipsoid circumscribing  $K$  and the maximum volume ellipsoid inscribed in  $K$  are two of the best known ellipsoids associated with  $K$ . The ellipsoids inherit any symmetry properties of the underlying body  $K$ . In this talk, we concentrate on the symmetry properties of these ellipsoids (and some others). Among others, we are interested in (a) investigation of how the symmetries of a body  $K$  influences some of its geometric characteristics, (b) explicit computation of the ellipsoids for classes of convex bodies  $K$  which have special symmetry properties, (c) classification of convex bodies with special symmetry properties, (d) using all these results to develop efficient algorithm for optimization problems.

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### MS17

#### **Optimization of Model and Computational Parameters in Expensive Engineering Simulations**

This talk describes our efforts to reduce computational time in optimization problems that require expensive engineering simulations. It is motivated by a class of problems in which each function evaluation requires both a Navier-Stokes hydrodynamic simulation process and an image registration process to recover from a reference image of a fluid certain unknown model parameter values. In the suggested approach, computational parameters, such as the grid size of the underlying simulation are treated as variables so that the fidelity of the simulation can be relaxed during

the optimization process, thus saving computational time. Surrogate functions are formed both on function values and on computational times and used in a way that pushes the optimization process to less expensive regions of the domain. Numerical results show that this approach has great potential for handling these types of problems.

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### MS17

#### **Some New Results in Derivative Free Optimization**

I am hoping they are new so I don't know what they are yet!

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### MS17

#### **Towards Multi-Objective Optimization Using Direct Search**

This talk presents a direct search algorithm for multi-objective optimization that finds a Pareto set solution for problems that are either unconstrained or subject to linear constraints. A Pareto solution set gives a number of solution alternatives that aim to represent the relative trade-off between several objectives. We also show that the approach is well suited for parallelization. We give numerical results for this method on a small set of problems.

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### MS17

#### **Issues of Polynomial Regression and Noisy Functions in Derivative Free Optimization**

Derivative free optimization methods are known to be reasonably successful in dealing with noisy black box functions. However, most of the theory of derivative free optimization so far was developed in the absence of noise. We will discuss theoretical issues that arise from considering noisy function. In particular, we will discuss how the conditions on sampling sets change when one uses polynomial regression rather than interpolation.

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**MS18**

### **Rational Learning in Networks**

We study a model of rational learning for self-interested agents embedded in an arbitrary network topology. We assume that there is an unknown state of the world, which the agents are trying to learn based on their private information about the state and their observations of the actions of their neighbors. We provide an explicit characterization of the perfect Bayesian equilibria of this dynamic game. We establish conditions on network topologies and private information structures under which agents can asymptotically learn the state of the world.

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**MS18**

### **Distributed Algorithms for Generalized Nash Games and Their Convergence**

We describe a distributed algorithm for a Nash equilibrium in a noncooperative game where each player's objective function and constraints both depend on the rival players's strategies.

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**MS18**

### **Pricing in Oligopoly Markets for Perishable Products: Learning and Loss of Efficiency**

In this talk we present a model for dynamically pricing multiple perishable products that sellers need to sell over a finite time horizon (i.e. in this setting, each seller has a fixed inventory of several products that he/she needs to sell over a finite time horizon). We are considering an oligopolistic market and assume that sellers compete through pricing (Bertrand competition). Applications in mind include pricing airline tickets in the face of competitor airlines, as well as selling seasonal products in the retail industry in the presence of competitors. The goal of this work is to address the competitive aspect of the problem but also the presence of demand uncertainty. In particular, we propose a model that uses ideas from quasi-variational inequalities (in order to address the aspect of competition), ideas from robust optimization as well as MPECs (in order to address "uncertainty" of the demand). Robust optimization allows us to propose a model that is tractable and does not assume any particular type of distribution for the uncertain parameters of demand. We consider open and closed loop policies through adjustable robust optimization. Furthermore, we consider a setting where sellers learn their demand price function parameters. Sellers only know that their demand belongs in a parametric class of demand functions. In this

setting there are two levels of learning: i) sellers learning their demand through data and ii) trying to understand their competitors' policies as they collect more data on prices for them and their competitors as time progresses and the selling horizon unfolds. We use ideas from MPECs to study this enhanced model of joint pricing and demand learning. (parts of this work are joint with S. Kachani, R. Lobel, D. Nguyen, A. Sood, C. Simon)

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**MS18**

### **Polynomial Stochastic Games Via Sum of Squares Optimization**

Stochastic games are an important class of games that generalize Markov decision processes to game theoretic scenarios. We consider finite state two-player zero-sum stochastic games over an infinite time horizon with discounted rewards. The players are assumed to have infinite strategy spaces and the payoffs are assumed to be polynomials. In this paper we restrict our attention to a very special class of games for which the single-controller assumption holds. It is shown that minimax equilibria and optimal strategies for such games may be obtained via semidefinite programming.

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**MS19**

### **Topology Optimization in Sheet Metal Design with Mixed-Integer Programming**

The design process of a multi-channel conduit involves a topology optimization in the first place. The question is how to arrange the different channels so that certain design goals such as minimum weight and/or maximum stability are met. We present different mixed-integer linear programming formulations for this problem, theoretical results, and numerical solutions for some test instances.

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**MS19**

### **Handling Manufacturing Constraints Using Discrete Optimization**

Given a topology of a sheet metal profile, how can it be produced when taking manufacturing restrictions into account? We model the problem as a graph such that each possible way of production corresponds to a Steiner tree. The manufacturing restrictions can be modeled as addi-

tional restrictions such as on the diameter or the degree of the tree. We present a mixed-integer program including all these constraints and develop new graph algorithms for its solution.

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## MS19

### New Forming Technologies for Sheet Metal

The processes linear flow splitting and linear bend splitting enable the production of branched profiles in integral style made of sheet metal without joining, lamination of material or heating of the semi-finished product. This new forming technologies provides the opportunity to design new product classes with optimized mechanical properties. By a following forming process new multi-chambered structures and integral stringer construction can be realized with thin walled cross-sections made from steel of higher strength.

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## MS19

### Product Properties as the Basis for Optimization

Product development can be seen as the optimization of internal properties (e.g. geometrical properties) to fulfil desired external properties (e.g. deflection of a beam). This approach needs precisely defined relations between external and internal properties based e.g. on physical models. These formalized interrelationships are used by subsequent mathematical optimization processes to compute and evaluate new geometries. We demonstrate our method by designing a multi-channel profile, which can for instance be used as a conduit.

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## MS20

### Optimum Active Pricing for Communication Networks with Multiple User Types and Information Asymmetry

The talk will introduce a class of hierarchical games that arises in pricing of services in communication networks

with a monopolistic service provider and a large population of users of different types. The probability distribution on different user types is common/public information, but the precise type of a specific user is not necessarily known to all parties. As such the game falls in the class of games with incomplete information, and in our specific case what we have is a problem of mechanism design within an uncertain environment and with asymmetric information. The service provider is a revenue maximizer, with his instrument being the prices charged (for bandwidth) as a function of the information available to him. The individual users are utility maximizers, with bandwidth usage being their decision variable. The congestion cost in their utility functions creates a coupling between different users' objective functions, which leads to a noncooperative game at the lower (users) level for which we adopt Nash or Bayesian equilibrium. Solutions to these problems (at both the lower and the upper levels) entail non-standard multi-level optimization problems. Indirect approaches to these optimization problems will be presented, and some asymptotics for large agent-population models will be discussed. (This is based on a joint work with Hongxia Shen.)

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## MS20

### Game Theoretic Approaches for Wireless Spectrum Sharing

Abstract not available at time of publication.

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## MS20

### From Optimization Theory to High-Speed Internet Access: An Overview of Power Control in Wireless and DSL Networks

This is an overview talk about the mathematical challenges and practical implications of optimization problems in interference-limited communication systems, including power control in wireless cellular networks and spectrum management in DSL broadband access networks. We will organize the wide range of results over the last 15 years in this area, illustrate the optimization-theoretic aspect of the problems, discuss the open problems in operational networks today, and highlight the interactions between the mathematics of convexity, algorithms, and games, and the engineering for the grande challenge of delivering high-speed communication access to as many users as possible.

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## MS20

### Optimization for Spectrum Management in Multiuser Communication

Optimal spectrum management in a communication system with multiple interfering users and hostile jammers is a major engineering design issue that has received considerable attention in both the optimization and electrical

engineering communities. From the optimization perspective, it provides a rich contemporary application context for innovative optimization, game theoretic, and economic modeling research as well as rigorous analysis. In this talk, we present an introduction to this area, focussing on formulation, complexity, asymptotic strong duality and polynomial time approximation.

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**MS21**  
**Failure of Newton-Like Methods for Optimization**

Global convergence analysis of unconstrained optimization methods usually involves making sure the Hessian approximation is bounded away from singularity. However, in practice methods for regularizing Newton-like methods often do bother with this issue. Our investigations into the behavior of Newton-like methods when the Hessian approximation approaches singularity show that failure due to singularity can occur only under very restricted circumstances. These results shed new light on several methods including the regularized Newton's method, the modified Cholesky factorization, and the Gauss-Newton method.

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**MS21**  
**Adaptive Cubic Regularisation Methods for Non-linear Optimization with Convex Constraints**

The adaptive cubic overestimation algorithm described in Cartis, Gould and Toint (2007) is adapted to the problem of minimizing a nonlinear, possibly nonconvex, smooth objective function over a convex domain. Convergence to first-order critical points is shown under standard assumptions, but without any Lipschitz continuity requirement on the Hessian of the objective. A worst-case complexity result for the Lipschitz continuous case is derived for a variant of the proposed method, which extends the best known bound for general unconstrained problems to nonlinear problems with convex constraints. Some preliminary numerical results are also presented.

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**MS21**  
**Matrix-Free Methods for PDE-Constrained Optimization**

Very large-scale nonlinear programming applications require careful selection of the most efficient numerical techniques. Prominent examples include problems where the constraints are defined by a discretized system of partial differential equations, such as shape optimization problems in Navier-Stokes flows. In this talk we consider the potential for the application of state-of-the-art optimization techniques to problems of this type.

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**MS21**  
**Parallel Optimization and the Toolkit for Advanced Optimization**

We begin by presenting information on the design and implementation of the Toolkit for Advanced Optimization (TAO), and how the reuse of common optimization components is facilitated within the framework. We then discuss some of the algorithms bundled with TAO for solving complementarity and optimization problems. Results for these methods are given along with an indication of their parallel performance.

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**MS22**  
**Applications of MPECs for Dynamic Optimization of Chemical Processes**

Switching conditions and nonsmooth models in the dynamic optimization of chemical engineering systems can be treated through the formulation of differential variational inequalities. In this talk we apply a temporal discretization to these dynamic systems and reformulate the variational inequalities to complementarity conditions and solved with NLP formulations for MPECs. Several chemical engineering examples are presented that illustrate these concepts.

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**MS22**  
**Feedback Solutions for Nonlinear Optimal Control Problems**

Optimal closed-loop (feedback) controllers, like the classical Linear Quadratic Regulator (LQR), are able to com-

pensate perturbations appearing in reality. Unfortunately these controllers are often designed for linear models only and hence are not optimal if the dynamical system appears nonlinearly. If these controllers are applied in a real process, the possibility of further data disturbances force recomputing the feedback control law in real-time to preserve stability and optimality, at least approximately. For this purpose, a new feedback method based on the parametric sensitivity analysis of NLP-problems is suggested. The new optimal controller can be adapted within a few nanoseconds on an typical personal computer.

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## MS22

### Optimal Control of Large Power Generating Kite Systems

We show how advanced dynamic optimization techniques based on Bock's direct multiple shooting method can be used to treat a challenging application problem, namely the periodic control of large, fast flying kite systems. After an outline of the technological idea we first show how to formulate the periodic optimal control problem for power generating kites, and how to estimate realistic model parameters based on measurement data. Second, we discuss several ways to control the kites in the presence of disturbances, among them a periodic linear control, and model predictive control. This is joint work with Boris Houska, Andreas Ilzhoefer, Kenny Evers, Bart Struyven.

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## MS22

### Semi-Automatic Transition from Simulation to Optimization

The talk concerns the development of mathematical methods, algorithmic techniques and software tools for the transition from simulation to optimization. The methodology is applicable to all areas of scientific computing, where large scale governing equations involving discretized PDEs are treated by custom made fixed point solvers. To exploit the domain specific experience and expertise invested in these simulation tools we propose to extend them in a semi-automated fashion. First they are augmented with adjoint solvers to obtain (reduced) derivatives and then this sensitivity information is immediately used to determine optimization corrections. In other words, rather than applying an outer optimization loop we prefer the "one-shot" strategy of pursuing optimality simultaneously with the goals of primal and adjoint feasibility. First results for aerodynamic shape optimization will be presented.

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## MS23

### Nested Approach for Solving Design Optimization Problem

Our talk concerns a design optimization problem, where

the constraint is a state equation that can only be solved by a typically rather slowly converging fixed point solver. This process can be augmented by a corresponding adjoint solver, and based on the resulting approximate reduced derivatives, also an optimization iteration, which actually changes the design. To coordinate the three iterative processes, we consider an augmented Lagrangian function that should be consistently reduced whatever combination of sequence of primal, dual and optimization steps one chooses. This function depends on weighting coefficients which involve the primal and dual residuals and on the Lagrangian. The key question is the choice of the weighting coefficients and the construction of the preconditioner in order to get a reasonable convergence rate of the coupled iteration. In this talk, we present theoretical results as well as some numerical results done by considering the Bratu equation on the 2D unit square.

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## MS23

### An SQP Method for Semilinear Elliptic Optimal Control Problems with Nonlinear Boundary Control-State Constraints

In this talk we will consider a family of optimal control problems governed by semilinear elliptic partial differential equations (PDEs) with pointwise nonlinear control-state inequality constraints. Problems with mixed control-state constraints are important as Lavrentiev-type regularizations of pointwise state-constrained problems, but they are also interesting in their own right. We will briefly review the associated optimality conditions and regularity results for Lagrange multipliers. Optimal control problems involving semilinear PDEs can be efficiently solved using the sequential quadratic programming (SQP) method, which is equivalent to a generalized Newton's method. The local convergence behavior of this method relies essentially on the strong regularity of the first-order optimality system, i.e., on the Lipschitz continuous behavior of solutions to an auxiliary linear-quadratic optimal control problem. Such Lipschitz stability results and the local quadratic convergence of the SQP method applied to the original problem will be discussed. Numerical examples will be used to illustrate our results.

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## MS23

### An Inexact SQP Method for Optimizing of a Simulated Moving Bed Process

The Simulated Moving Bed process is an adsorption process for the separation of dissolved chemicals. It consists of several cyclically connected adsorption columns. By means of periodical switching of inflow and outflow ports between the columns, a counter-current movement of the adsorbent is simulated. When operated over a longer time, the process runs into a cyclic steady state (CSS). Desirable is a CSS which is optimal with respect to operational costs and product specifications. This can be modelled as a PDE constrained optimization problem with periodicity constraint in time. An inexact SQP method is used solve the discretized optimization problem. Inspired from

so called Newton-Picard methods for calculation of the CSS, only low-rank approximations of the periodicity constraint derivative are calculated, requiring only few directional derivatives. An orthogonal basis of an approximation to the eigenspace of the largest eigenvalues of the periodicity constraint jacobian is simultaneously updated by a Subspace Iteration to yield the derivative directions.

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### MS23

#### **On a State-Constrained Optimal Control Problem Involving Nonlocal Radiation Interface Conditions**

A state-constrained optimal control problem arising in the context of sublimation crystal growth is considered. The nonlocal radiation interface conditions and the presence of pointwise state-constraints constitute a major issue of this problem. The goal of this talk is twofold: Firstly, the necessary and sufficient optimality conditions associated with the problem are discussed. Secondly, a Moreau-Yosida type regularization is considered to cope with the weak regularity of the Lagrange multipliers. Optimality conditions for the regularized problem are presented and the convergence of the regularized solutions is shown.

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### MS24

#### **A Backtracking Heuristic for Graph Coloring**

The number of colors used by a greedy graph coloring algorithm is to a large extent determined by the order in

which the vertices are colored. We present a backtracking correction algorithm that partially changes the effects of the underlying vertex ordering by rearranging the mapping of the colors. The backtracking heuristic is used in conjunction with a top level coloring algorithm to decrease the number of colors in the graph.

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### MS24

#### **Heuristics for the Linear Arrangement Problem**

The linear arrangement minimization problem consists of finding a labeling or arrangement of the vertices of a graph that minimizes the sum of the absolute values of the differences between the labels of adjacent vertices. This is a well-known NP-hard problem that presents a challenge to solution methods based on heuristic optimization. Many linear arrangement reduction algorithms have recently been developed and applied to structural engineering, VLSI and software testing. We undertake the development of different heuristic procedures with the goal of uncovering the most effective designs to tackle this difficult but important problem. Specifically, we consider the adaptation of constructive, local search, GRASP and Path Relinking methods for the linear arrangement minimization. We perform computational experiments with previously reported instances to first study the effects of changes in critical search parameters and then to compare the efficiency of our proposal with previous solution procedures.

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### MS24

#### **Minimal Arrangement of Clos Networks**

Clos networks are switching matrices that are used in high frequency transmissions. For a given matrix with N inputs and M outputs, these matrices are arranged in three stages each of which is build up by so-called switches. Whereas the size and number of switches in the first and third stage are basically determined by N and M the task is to find the minimal number of switches in the middle stage. How many of these switches are necessary to guarantee routability is a long open question even for small sized matrices. By applying techniques from integer and combinatorial optimization we are able to determine the minimal number of switches for Clos networks with up to 32 inputs and outputs.

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#### MS24

##### 0/1 Model for the Linear Arrangement Problem

The Linear Arrangement Problem consists of finding an ordering of the nodes of a weighted graph on  $n$  nodes such that the sum of the weighted edge lengths is minimized. We report about the usefulness of a new modeling approach within a branch-and-cut algorithm for solving Linear Arrangement Problems to optimality. The key idea is to introduce binary variables  $d_{ijk}$  for  $1 \leq i < j \leq n$  and  $1 \leq k \leq n - 1$ , where  $d_{ijk} = 1$  if nodes  $i$  and  $j$  have distance  $k$ . We present different strategies how the number of variables within this model can be reduced.

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#### MS25

##### On the Nullstellensatz Method for Combinatorial Optimization

Unlike linear models, systems of multivariate polynomial equations over the complex numbers can be easily used to model combinatorial problems. In this way, a problem is feasible (e.g. a graph is 3-colorable, Hamiltonian, etc.) if and only if a certain system of polynomial equations has a complex solution. In the work of M. Laurent, J. Lasserre and P. Parrilo, Y. Nesterov, and others, optimization problems which are modeled by a zero dimensional radical ideal have been shown to have a finite sequence of semidefinite programs that converge to the optimal solution. But for feasibility problems (e.g., is  $G$  Hamiltonian?) the (complex) Hilbert Nullstellensatz gives a sequence of *linear algebra* problems that eventually decides for sure the property. In this talk we present theoretical and experimental results about these sequences of linear algebra relaxations to the combinatorial optimization problem. We show that the size of the smallest Nullstellensatz linear algebra system certifying that there is no stable set of size larger than the stability number of the graph grows as fast as the stability number of the graph. We also show discuss this method as a practical way for detecting 3-colorability of graphs.

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#### MS25

##### Finding Low-Rank Matrices by Convex Optimization

In many applications, notions such as complexity or degree of a model or design correspond to the rank of a matrix. Choosing the “simplest” model often results in a matrix rank minimization problem, which is NP-hard in general. This talk discusses convex relaxations based on semidefinite programming, and covers recent results on guaranteed minimum rank solutions to linear equalities via nuclear norm minimization.

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#### MS25

##### Semidefinite Programming with Matrix Variables

The talk describes progress with algorithms which take advantage of matrix structure. They start symbolically with noncommutative algebra and derive efficient expressions for the linear subproblem. Then they proceed with iterative numerical linear solvers.

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#### MS25

##### Semidefinite Programming Approach for Polynomial Least Squares Problems

We consider solving polynomial least squares problems via semidefinite programming relaxation. The degree of the objective function, represented as a sum of positive and even powers of polynomials, affects the computational efficiency. We propose the methods to transform polynomial least squares problems to polynomial semidefinite programs to reduce degrees of the polynomials. The efficiency of solving the original polynomial least squares problem and the transformed polynomial semidefinite programs is compared. Numerical results on selected polynomial least squares problems show better performance of the transformed polynomial semidefinite program.

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#### MS26

##### Intriguing Analogies Between the Edge and Central Paths

Linear optimization consists of maximizing, or minimizing, a linear function over a domain defined by a set of linear inequalities. Simplex methods, which follow an edge-path, and the primal-dual interior point methods, which follow the central path, are currently the most computationally successful algorithms. In this talk we highlight intriguing analogies between the edge and central paths, and between the diameter of a polytope and the largest possible total curvature of the associated central path.

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#### MS26

##### A Comparative Study of Notions of Curvature of Central Path in Linear Programming

The central path method is one of the most efficient in-

terior point methods to solve linear programs. Recently, several attempts have been made to study the geometry of central path, particularly, the curvature of central path using different notions of curvature. In this paper we present a comparative study of various notions of curvature of central path in linear programming.

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## MS26

### Curvature of Central Path and Computational Complexity of Linear Programming

In this paper we present some new results to develop bounds on the curvature of the central path of a linear program (LP), and use them to obtain upper and lower bounds, in the form of curvature integral, on the iteration complexity of LP path following algorithms.

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## MS26

### An Information Geometric Approach to Polynomial-Time Interior-Point Algorithms: Complexity Bound Via Curvature Integral

We study polynomial-time interior-point algorithms in view of information geometry. We consider information geometric structure for conic linear programs introduced by self-concordant barrier functions, and develop a precise iteration-complexity estimate based on an integral of curvature of the central trajectory in a rigorous differential geometrical sense. The theory has a surprising link to the existing results on geometrical structures of the central trajectory for classical LP by Vavasis and Ye, and Monteiro and Tsuchiya.

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## MS27

### Considerations in Evaluating Derivative-Free Methods for Simulation-Based Optimization Problems

Derivative-free methods have emerged as invaluable for finding solutions to simulation-based optimization problems. However, one must consider that the goal in solving such problems may not be to merely find the classical

”best” solution (i.e. the point that results in the smallest function value) but may also include finding a solution which is robust with respect to the simulator. For example, it may be the case that answer A gives a smaller objective function value, but that answer B is preferable in real world situations. Moreover, efficiency is important because the optimization is guided solely by function values which require the solution of a simulation. In this talk, we will examine these and other considerations that must be taken into account when optimization methods are evaluated for their usefulness and effectiveness. We will also discuss appropriate metrics for making comparisons between methods.

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## MS27

### Accelerating Active Set Methods and Extensions to DFO.

In this talk we explore new strategies to accelerate active set methods. We devote the second part of the talk to discuss the implications for methods that do not make use of derivatives.

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## MS27

### Benchmarking Algorithms for Derivative-Free Optimization

Performance profiles have proven to be a useful tool for comparing algorithms on large sets of problems in the derivative-based optimization setting. We introduce two new complementary performance measures – relying only on function values – which address the different computational budgets and desired accuracy-levels found in derivative-free optimization. We illustrate the use of the new benchmarking procedures by comparing several derivative-free optimization algorithms on a new set of test problems.

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**MS27****Testing, Testing, 1, 2, 3—Do We Really Know How?**

Many experts in areas ranging from system software to direct marketing assert that testing is a science. If they are correct, it is fair to ask whether experts in non-derivative optimization are prepared to make definitive statements about (i) which methods are the best choice for various problem classes, and (ii) which implementations are the most effective and reliable. Since getting non-controversial answers to these questions remains problematic, this talk will examine our current knowledge about the computational properties and practical performance of non-derivative optimization methods, and also consider whether we can define sensible metrics to enhance future testing.

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**MS28****An Adaptive Retrospective Trust-Region Algorithm for Stochastic Programming**

Bastin et al. have recently proposed a variant of the classical trust-region, called retrospective trust-region. Its main ingredient is that the trust-region radius update is decided based on the retrospective ratio between the current iterate and the previous one. In this talk, we exploit this idea inside the adaptive trust-region method developed by Bastin, Cirillo and Toint for nonlinear stochastic programming, also using this ratio when deciding the level of accuracy of sample average approximations.

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**MS28****Decomposition Schemes for Stochastic DVIs**

A recent paper by Pang and Stewart (2007) provides a comprehensive introduction to differential variational inequalities (DVI). We consider a stochastic generalization of such problems, looking specifically at uncertainty in the control problem within the DVI framework. Decomposition schemes for such problems are discussed and some preliminary algorithmic evidence is provided.

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**MS28****Stochastic Variational Inequalities: Models and Algorithms**

We consider the class of variational inequalities resulting from coupled two-period stochastic Nash games and discuss some motivating applications. Existence statements are provided in a variety of settings. Furthermore, we provide a discussion of chance-constrained VIs, a relatively new class of stochastic equilibrium problems. Some preliminary algorithmic efforts are discussed.

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**MS28****Adaptive Precision Adjustment in Stochastic Nonlinear Programming**

We consider nonlinear stochastic programs and present an approach for adaptively determining efficient sample sizes in sample average approximations. The approach uses rate of convergence and sampling error estimates to determine sample sizes for the next several iterations. The approach balances computational cost of large sample sizes with accuracy of the sample averages. The approach is implemented using a rolling planning horizon and is illustrated with applications from structural engineering design problems.

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**MS29****Multigrid One-Shot Pseudo-Time Stepping**

### Method for Aerodynamic Shape Optimization

This talk presents a numerical method for aerodynamic shape optimization problems. It is based on simultaneous pseudo-time stepping in which stationary states are obtained by solving the pseudo-stationary system of state, co-state and design equations. The main advantages of this method are that it blends in nicely with an existing pseudo-time stepping method for the state and the co-state equations, that it requires no additional globalization techniques in the design space, and that a preconditioner can be used for convergence acceleration which stems from the reduced SQP methods. To accelerate the convergence of the method further, 'optimization based' multigrid strategy can be implemented.

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### MS29

#### Aerodynamic Shape Optimization of an Oblique Flying Wing

Adjoint solvers for 3D computational fluid dynamics are extremely useful for performing aerodynamic shape optimization of aircraft configurations. A new adjoint approach is presented, where automatic differentiation is applied selectively to compute the partial derivatives present in the adjoint equations. This selective application of automatic differentiation is the central idea behind the ADjoint (automatic differentiation adjoint) approach. An implementation of this approach is used to optimize an oblique flying wing subject to trim constraints.

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### MS29

#### Error Estimation and Sensitivity Analysis for Fluid Flow Problems Involving Complex Geometries

The development of an adjoint method is presented for the computation of discretization error estimates and shape sensitivities of objective functions for aerodynamic design problems. The adjoint method is implemented in conjunction with an embedded-boundary Cartesian mesh approach. Several three-dimensional design examples, using aircraft and spacecraft configurations, are used to demonstrate the robustness and efficiency of the resulting optimization framework.

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### MS29

#### Toward Practical Application of Numerical Aerodynamic Optimization

An aerodynamic component, such as a wing, must function effectively under a range of on- and off-design operating conditions. Therefore, the associated aerodynamic optimization problem has many competing objectives. In this presentation, an automated approach to such problems is described and demonstrated. The basic idea is to treat the off-design operating requirements as constraints while the

on-design conditions are assigned weights based on their relative importance. The resulting constrained multi-point problem is solved using a gradient-based Newton-Krylov algorithm based on the discrete-adjoint approach.

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### MS30

#### Optimal Control in Image Processing for Breast Cancer Detection

Motivated by a problem in mammographic image processing, we develop a natural model for smooth image interpolation. The model is based on a class of degenerate parabolic PDEs as well as an optimal control problem associated with the variable degeneracies. The control variable enters the diffusion coefficients of the PDE and, implicitly, the solution space. We discuss spaces of discontinuous functions adapted to the PDE and the optimization problem. We further demonstrate how a characterization in terms of certain weighted and directional Sobolev spaces can be found which in turn enables us to obtain existence results for the simultaneous solution of the optimal control problem and the PDE.

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### MS30

#### Optimal Treatment Planning in Radiotherapy Based on Boltzmann Transport

Most dose calculation algorithms in clinical use rely on the Fermi-Eyges theory of radiation which is insufficient at inhomogeneities, e.g. void-like spaces like the lung. In contrast, this work is based on a Boltzmann transport model for the radiation which accurately describes all physical interactions. Starting with this model we develop a direct optimization approach using adjoint equations. Several numerical results are presented.

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### MS30

#### Constructing Vascular Systems from Optimality Criteria

We create realistic vascular systems based on optimality principles of theoretical physiology. Our technique takes as input the position and flow distribution of end points of a vascular system. Optimization is driven by intravascular volume minimization. Direct optimization of a vascular system, including topological changes, is used instead of simulating vessel growth. A good initial condition is found by extracting key information from a previously optimized model. This technique is used iteratively in a multi-level approach to create a more globally optimized vascular system. The generated models are similar to real data acquired from corrosion casts of a human liver.

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**MS31****An Interior-Point Piecewise-Penalty Method for Nonlinear Programming**

We present an interior-point penalty method for nonlinear programming (NLP), where the merit function consists of a piecewise linear penalty function (PLPF) and an  $\ell_2$ -penalty function. The PLPF is defined by a set of penalty parameters that correspond to break points of the PLPF and are updated at every iteration. The step direction is computed from an  $\ell_2$ -regularized Newton system of the first-order equations of the barrier problem. In line search, a trial point is accepted if it provides a sufficient reduction in either the PLPF or the  $\ell_2$ -penalty function. We establish strong global as well as fast local convergence properties of the algorithm. Encouraging numerical results on CUTER test set will be reported.

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**MS31****Infeasibility Detection in Nonlinear Programming**

One of the central questions in optimization is to determine if a problem is feasible. This question is important in its own right since it may be difficult for a modeler to know if the constraints imposed on a problem are compatible. Feasibility detection also plays a key algorithmic role in branch and bound algorithms for mixed integer nonlinear optimization. In that context, the problem has a special structure as it is known that only one constraint (or a group of constraints) has been added to a problem that is known to be feasible. In this talk we describe two new infeasibility detection techniques for nonlinear optimization based on penalty methods.

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**MS31****An Adaptive Cubic Overestimation Funnel Algorithm for Constrained Optimization**

In two recent papers, the authors have explored a novel adaptive cubic overestimation (ACO) algorithm for unconstrained optimization (with C. Cartis) and a non-standard trust-funnel algorithm for equality constrained problems. The first may be seen as an alternative globalization technique, with strong links with trust-region methods. The second uses two simultaneous trust-regions (in the range- and null-spaces of the constraints, respectively) together with a "funnel" to enforce global convergence to first-order stationary points. This talk will explore the natural cross-breed between those two proposals, in which two distinct cubic overestimators are adaptively computed in the range- and null-spaces of the constraints, in conjunction with a funnel and/or a filter.

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**MS31****Warm Starting Interior-Point Methods in Branch and Bound**

Interior-point methods are needed to solve continuous subproblems arising in large-scale, nonlinear mixed-integer programming. We will propose a specialized penalty approach for warm-starting interior methods inside branch and bound methods, where the continuous subproblems change in a very structured way. We will outline our penalty approach, present a theoretical summary of the approach, and present numerical results on sample problems.

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**MS32****Application of Large Scale Parameter Estimation in the Aerospace Industry**

Abstract not available at time of publication.

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**MS32****Fast Online Computation for Linear and Nonlinear Model Predictive Control in the kHz Range**

The powerful feedback control technique of model predictive control (MPC) is already widely applied in industries

with slow complex processes, like chemicals, where the on-line solution of optimal control problems is possible. With more efficient computation, MPC promises to revolutionize the way fast systems are controlled, e.g. in mechatronics and automotive applications. In these industries, explicit MPC approaches are until now popular, which precompute all solutions and avoid online optimization, but suffer severely from the curse of dimensionality and have a very limited range of applicability. This talk focuses on the question how the most efficient methods for nonlinear optimization in MPC, that have proven successful in chemical engineering applications, can be transferred to milli and microsecond applications. Several new issues pop up, e.g. how to efficiently solve online QPs, how to work with old system linearizations as long as possible, how to efficiently shift problem data and matrix factorizations, etc. Finally, we briefly present real-world and simulated MPC applications from automotive, mechatronic, and power engineering. This talk is based on joint work with Hans Joachim Ferreau, Leonard Wirsching, Lieboud Van Den Brouck, Andreas Ilzhoefer, Boris Houska.

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### MS32

#### Feature-Based Sensitivity Analysis and Parameter Estimation for Dynamical Systems

Methods for the sensitivity analysis of “features” of nonlinear dynamical systems are developed, in particular features of oscillatory systems (period, amplitude and phase). Then, the benefits of “feature-based” parameter estimation will be demonstrated in the context of models from cell and circadian biology. The resulting objective functions are well behaved and the available experimental data lends itself to the application of this technique. Finally, feature-based sensitivity analysis is applied for post-optimality sensitivity analysis.

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### MS32

#### Frameworks for Direct Transcription

We discuss a general framework for the simultaneous collocation method for the solution of dynamic optimization problems. Problems in this class include parameter estimation, optimal control, multistage optimization and even optimization with steady-state, distributed models. The talk explores the role of fast NLP algorithms, problem decompositions, NLP sensitivity and formulations to deal with

discrete decisions.

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### MS33

#### Large-Scale Parallel Algorithms for Inverse Problems in Electrocardiology

In this work, we consider an inverse problem for the estimation of the electrical properties of the heart tissue. We solve for the tissue excitability, a scalar spatial field that determines the propagation of the action potential in the myocardium. The Fitz-Hugh Nagumo model is a nonlinear, two species reaction-diffusion PDE that models the cardiac electrical activity. The inverse problem is formulated as a PDE-constrained optimization problem constrained by the Fitz-Hugh Nagumo model. We use an  $L^2$ -Tikhonov regularization for stability. We use a reduced space approach and eliminate the state and the adjoint variables, and iterate in the inversion parameter space using conjugate-gradient (CG) algorithm. We precondition CG by a V-cycle multigrid scheme where the smoother in the multigrid scheme is one application of a reduced Hessian preconditioner constructed using a appropriately selected Green’s function. We use operator splitting, a pseudo-spectral discretization for diffusion, and a backward Euler scheme to time-evolve the state and the adjoint equations. We present fixed size and iso-granular scalability results for problems with up to one billion variables on 1024 processors on a Cray XT3 at the Pittsburgh Supercomputing Center.

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### MS33

#### Domain Decomposition and Model Reduction for the Optimal Control of Systems with Local Nonlinearities

In several applications one is interested in the optimal control of systems in which nonlinear partial differential equations (PDEs) are posed on relatively small subdomains and are coupled to linear PDEs on surrounding, larger subdomains. The linear PDE solution on the surrounding subdomains needs to be computed accurately enough to provide acceptable boundary conditions for the nonlinear problem on the ‘inner’ subdomain. Our approach for solving such problems combine balanced truncation model reduction and optimization-ased domain decomposition to derive reduced order models with guaranteed error bounds for these PDE constrained optimization problems. Balanced truncation is applied to the linear subproblems with inputs and outputs determined by the original in- and outputs as well as the interface conditions between the subproblems. Optimization is applied to the reduced problems. The potential of this approach is demonstrated for model problems motivated by flow control and design applications.

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### MS33

#### The Smoothed Penalty Method for Inequality Constrained Optimal Control Problems

We present an infinite dimensional version of a smoothed-penalty method for inequality constrained optimization problems. The algorithm has been introduced by Spelucci et. al. for finite-dimensional quadratic programming problems. In finite dimensions it is based on smooth approximations to the exact  $l_1$ -penalty function. We extend it to the infinite-dimensional setting and derive estimates on the control of smoothing and penalty parameter. Using these estimates convergence of the sequence of iterates is proven. We report numerical results for examples of optimal control problems for partial differential equations with pointwise state constraints.

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### MS33

#### Solving State-Constrained Parabolic Optimal Control Problems by Level-Set Based Shape Optimization Techniques

In the construction of algorithms for the numerical solution of state constrained optimal control problems one usually has to deal with the structural problem that multipliers are singular measures which are concentrated on the boundary of the active set of the constraint. Algorithms using approximations of the multiplier, e.g., by approximate delta functions show a strong mesh dependence and can not easily be transferred into the infinite dimensional setting. Hintermueller and Ring used the idea of treating the active set as an unknown in a geometric shape space which needs to be identified in such a way that the optimality system is satisfied. The identification problem was formulated as a shape optimization problem and the optimal shape was found using a level-set based technique, with a preconditioned shape gradient acting as the driving force for the shape variable. It turned out that the singular multiplier is part of the obtained driving force. It is incorporated into the speed function for the propagation of the level-set function by using a standard extension procedure thus posing no further numerical difficulties. This shape optimization idea is now extended to the parabolic case. The active set then becomes time-dependent and has to be identified in each time-step. This means, the propagation of the level-set function takes place in the space-time cylinder and the direct and the adjoint equations have to be solved on non-cylindrical domains. The approach is carried out tested for the linear heat equation and for a non-linear coupled thermistor equation.

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### MS34

#### Tuning Parameters for Prediction in Regularized Kernel Estimation

The Regularized Kernel Estimation (RKE) framework was introduced by Lu et al. (PNAS 2006) as a robust method for estimating dissimilarity measures between objects from noisy, incomplete, inconsistent and repetitious dissimilarity data. The RKE framework is useful in settings where object classification or clustering is desired but objects do not easily admit description by fixed length feature vectors. Instead, there is access to a source of noisy and incomplete dissimilarity information between objects, usually described as a graph. RKE estimates a symmetric positive semidefinite kernel matrix  $K$  which induces a real squared distance admitting of an inner product.  $K$  is the solution to an optimization problem with semidefinite constraints that trades-off fit to the observed dissimilarity data and a penalty of the form  $J_{\lambda_{rke}}(K)$  on the complexity of  $K$ , where  $\lambda_{rke}$  is a non-negative regularization parameter. RKE uses the penalty  $J_{\lambda_{rke}}(K) = \lambda_{rke} \text{tr}(K)$ . We present results on methods for choosing values of the regularization parameter  $\lambda_{rke}$  in the RKE problem, in particular, when the solution  $K$  is then used in a prediction task. We show the CV2 method which selects regularization parameter values in clustering and visualization applications. However, based on an empirical study using protein sequence data, we make the observation that similar clustering performance is achievable for a range of values of the RKE regularization parameter, indicating that precise tuning in these applications might not be required. Based on the same empirical study we make the observation that prediction performance, in contrast to clustering, may be highly dependent on the RKE regularization parameter. We provide initial results on methods that jointly tune regularization parameters in both the RKE and prediction optimization problems.

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### MS34

#### An Improved SDP-Based Distributed Algorithm Forgraph Realization with Applications to Molecular Conformation

We propose an algorithm for determining a protein molecule structure given sparse and noisy short-range interatom distances. Our divide-and-conquer algorithm recursively partitions the atoms into overlapping groups; estimates via a semidefinite program and refines via gradient descent groups with fewer than 300 atoms; finally stitches overlapping groups to form the protein configuration. The algorithm is tested on molecules taken from the PDB database. A 13000-atom conformation problem is solved in 3 hours with an RMSD of 1.0Å, given 30% of

the distances less than  $6\text{\AA}$ .

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#### MS34

##### **Attacking the Nonconvexity of Graph Embedding Directly, With Application to Molecular Conformation**

We discuss an approach to graph embedding that leads to a matrix optimization problem with nonconvex rank constraints. Rather than solve a convex semidefinite relaxation of the rank constraints we attack them directly using straightforward nonlinear programming techniques. Our approach has proven successful when applied to the embedding problem in molecular biology. We discuss the computational issues that arise, numerical experience with the embedding problem, and alternative problem formulations based on nonconvex duality principles.

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#### MS34

##### **A Brief History of Embedding**

Graph embedding problems appear in many guises. In the 1950s and 1960s, psychometricians and statisticians developed *multidimensional scaling*, a collection of techniques for visualizing proximity data in low-dimensional Euclidean spaces. These techniques can be understood as algorithms for minimizing some measure of discrepancy between a set of Euclidean distance matrices and a set of dissimilarity matrices. Modern applications of graph embedding, e.g., inferring 3-dimensional molecular structure from information about interatomic distances, assigning locations to a network of sensors, various techniques for *manifold learning* (nonlinear dimension reduction of multivariate data), can be formulated in the same manner.

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#### MS35

##### **On the Road to Tractability: From Combinatorial Optimization Via Copositive Programming to SDP-Based Approximation**

Quite many combinatorial and some important non-convex continuous optimization problems admit a copositive representation, where the complexity of solving discrete, or non-convex, programs is shifted towards the complexity of sheer feasibility. Using characterizations of copositivity, one arrives at various SDP-based approximations. However, not all of these are tractable with current technology. This talk addresses some approaches on which tractable SDP approximations may be based, along with specific strategies to generate interesting test instances of intermediate

complexity.

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#### MS35

##### **On Semidefinite Programming Relaxations of the Travelling Salesman Problem**

We review known results on semidefinite programming (SDP) relaxations of the traveling salesman problem (TSP). Subsequently, we introduce a new SDP relaxation of TSP based on an SDP relaxation of the quadratic assignment problem. We also present and analyse a randomized rounding procedure that produces a tour from the optimal SDP solution. The relaxation and rounding procedure will be illustrated on numerical examples.

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#### MS35

##### **Sensor Network Localization, Euclidean Distance Matrix Completions, and Graph Realization**

We study Semidefinite Programming, SDP, relaxations for Sensor Network Localization, SNL, with anchors and with noisy distance information. The main point of the paper is to view SNL as a (nearest) Euclidean Distance Matrix, EDM, completion problem and to show the advantages for using this latter, well studied model. We first show that the current popular SDP relaxation is equivalent to known relaxations in the literature for EDM completions. The existence of anchors in the problem is not special. The set of anchors simply corresponds to a given fixed clique for the graph of the EDM problem. We next propose a method of projection when a large clique or a dense subgraph is identified in the underlying graph. This projection reduces the size, and improves the stability, of the relaxation.

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#### MS35

##### **Strong Duality and Stability in Conic Convex Programming**

For nonlinear (minimization) optimization problems with optimal value  $v_P$ , *weak duality* holds in general, i.e. the optimal value of the Lagrangian dual provides a lower bound,



$v_D \leq v_P$ . However, *strong duality* (i.e.  $v_D = v_P$  and  $v_D$  is attained) requires a *constraint qualification*, CQ, e.g. the Slater (strict feasibility) CQ. In the absence of a CQ, the dual optimal value  $v_D$  may be unattained and/or there can be a positive duality gap  $v_P - v_D > 0$ . In addition, the (near) absence of a CQ results in numerical difficulties.

We study conditions that guarantee a finite positive duality gap  $\infty > v_P - v_D > 0$ . Necessary and sufficient conditions for a finite nonzero duality gap are given, and it is shown how these can be used to generate instances satisfying this property. Numerical tests are included. We then present an algorithm that solves in an efficient and stable way, feasible conic convex optimization problems, including those for which the Slater constraint qualification fails. In addition, we illustrate the close relation between strict complementarity and duality gaps.

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### MS36

#### Using Nonnegative Matrix and Tensor Factorizations for Topic Detection and Tracking

The automated identification of semantic features is an important goal for text mining applications. Through the use of low-rank nonnegative matrix factorization (NNMF), one can retain natural data nonnegativity and thereby eliminate the need for subtractive basis vector and encoding calculations common to approaches such as principal component analysis for semantic feature abstraction. With appropriate extensions, nonnegative tensor factorization (NNTF) can be used to exploit both temporal and semantic proximity and enable tracking of text-based objects from a variety of media. Exposing latent (unknown) communication patterns within social networking environments, for example, would be possible with NNTF-based models. Demonstrations of NNMF and NNTF algorithms for topic (or discussion) detection and tracking using corpora such as the Enron Email dataset will be presented.

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### MS36

#### Effective Initializations for NMF algorithms

Nonnegative Matrix Factorization approximates a nonnegative matrix  $A \in \mathbb{R}^{m \times n}$ , as  $A \approx WH$ , for two nonnegative

matrices  $W \in \mathbb{R}^{m \times k}$  and  $H \in \mathbb{R}^{k \times n}$ , and some  $k \ll n$ . Existing algorithms typically start from random  $W$  and  $H$  and iterate until convergence. This type of initialization typically causes slow convergence, making the overall process quite expensive. In this talk we present alternative, typically more efficient, initialization techniques for NMF and its one sided variants, where there is no restriction in the sign of one of the two factors. This presentation is joint work of C. Boutsidis (RPI) and E. Gallopoulos (U. Patras).

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### MS36

#### Nonnegative Matrix Factorizations and Clustering

Variations of the Nonnegative Matrix Factorization (NMF) are discussed for their application to clustering. We show how interpreting the objective function of K-means as that of a lower rank approximation with special constraints allows comparisons between various formulations of NMF and K-means and provides the insight to design new clustering algorithms. We discuss introduction of additional constraints such as sparsity and orthogonality on the factors in the NMF objective function for the purpose of designing clustering algorithms based on NMF. The experimental results with synthetic and text data shows that these constrained NMF algorithms not only provide an alternative to K-means, but rather give much better and consistent solutions to the clustering problem.

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### MS36

#### Greedy Algorithms and Complexity for Nonnegative Matrix Factorization

Nonnegative matrix factorization has become an important tool in data mining. This talk will cover a class of algorithms called 'greedy downdating' and will show that they are effective for simple models of text databases. We will also show that NMF is an NP-hard problem in general.

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### MS37

#### A Subclass of Generating Set Search with Second-Order Convergence

We introduce a general subclass of generating set search algorithms, in which approximate second derivative information based only on previously sampled points is used to

construct directions for the algorithm to use. Specifically, if we have an approximate Hessian at each iteration, we choose as directions its orthonormal eigenvectors and their negatives. We show that if the sequence of approximate Hessians converges to the true Hessian in the limit, convergence to second-order stationary points can be achieved. We then discuss specific implementations for approximating the Hessian in a way that can satisfy the hypotheses of the convergence theory. We conclude by presenting some numerical results that verify our approach.

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### MS37

#### Advancements in the Development of HOPSPACK

HOPSPACK facilitates hybrid optimization using native source code of existing software. Two levels of parallelism are supported; both function evaluations and individual optimizers may run asynchronously in parallel using a communal function value cache. Load balance is exploited to create efficient hybrids that share information, improving overall robustness. A simple interface allows users to dynamically build custom combinations of supported optimizers. We will provide numerical results to demonstrate the overall effectiveness of parallel hybrid optimization.

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Recent developments in generating set search for n

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### MS37

#### Sequential Penalty Approaches for Nonlinear Constrained Optimization Without Derivatives

We consider the problem of minimizing a continuously differentiable function subject to smooth nonlinear constraints. We assume that the first order derivatives of the objective function and of the constraints are not available. In this work we propose new globally convergent pattern search and linsearch methods which are based on smooth sequential penalty functions. Numerical results on standard test problems and the computational experience on a practical problem show that the approach is viable.

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### MS37

#### Recent Developments in Generating Set Search for Nonlinear Programming

Recent experiments with generating set search (GSS) have made clear that careful implementation choices can have an appreciable impact on the performance of GSS methods, in terms of both reducing the number of function and constraint evaluations required to find improvement and keeping the computational overhead of the algorithm at a minimum. Furthermore, analysis provides useful insights when making such choices. In this talk we will discuss further developments along this front.

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### MS38

#### Sampling and Integer Programming for Chance-Constrained Problems

Various applications in reliability and risk management give rise to optimization problems with constraints involving random parameters which are required to be satisfied with a pre-specified probability threshold. There are two main difficulties with such chance-constrained problems. First, checking feasibility of a given candidate solution exactly is, in general, impossible since this requires evaluating quantiles of random functions. Second, the feasible region induced by chance constraints is, in general, non-convex leading to severe optimization challenges. We address the first difficulty by solving approximate problems based on Monte Carlo samples of the random data. We demonstrate that this scheme can be used to yield both feasible solutions and statistical optimality bounds using modest sample sizes. Computational testing of the sampling approach indicates that it can be used to yield good feasible solutions and reasonable bounds on their quality. We address the second difficulty via integer programming. We perform a detailed polyhedral study of the convex hull of the set of feasible solutions of such problems, and develop families of strong valid inequalities. These inequalities, when used within a branch-and-cut scheme, serve to significantly improve relaxation bounds, and expedite convergence, hence allowing instances that are considerably larger than have been considered before to be solved to optimality. (Based on joint work with James Luedtke and George L. Nemhauser)

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**MS38****Optimization Problems with Multivariate Stochastic Ordering Constraints**

We consider stochastic optimization problems where risk-aversion is expressed by a stochastic ordering constraint. The constraint requires that a random vector depending on our decisions stochastically dominates a given benchmark random vector. We identify a suitable multivariate stochastic order and describe its generator in terms of von Neumann–Morgenstern utility functions. We develop necessary and sufficient conditions of optimality and duality relations for optimization problems with this constraint. Assuming convexity we show that the Lagrange multipliers corresponding to dominance constraints are elements of the generator of this order, thus refining and generalizing earlier results for optimization under univariate stochastic dominance constraints. Furthermore, we obtain necessary conditions of optimality for non-convex problems under additional smoothness assumptions.

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**MS38****Combinatorial Pattern Method for Probabilistically Constrained Optimization Problems**

I consider stochastic optimization problems containing a joint probabilistic constraint with a random right-hand side following a multivariate probability distribution with finite support. I propose a novel approach based on the extraction of combinatorial patterns that define the minimal conditions to be satisfied for the joint probabilistic constraint to hold. The combinatorial patterns take the form of conjunctions of literals and the probabilistic constraint is replaced by a constraint on a disjunctive normal form. The approach allows the substitution of an MIP for the original stochastic problem. Computational results will be presented.

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**MS38****Cutting Plane Methods for Optimization Problems with Stochastic Dominance Constraints**

For stochastic optimization problems with second order stochastic dominance constraints we present two formulations involving small numbers of variables and exponentially many constraints: primal and dual. The dual formulation reveals connections between dominance constraints, generalized transportation problems, and the theory of measures with given marginals. Both formulations lead to two classes of cutting plane methods. Convergence of both methods is proved in the case of finitely many events. Numerical results for a portfolio problem are provided.

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**MS39****Formulations for Supersonic Design Optimization**

State-of-the-art design of supersonic aircraft has relied on inverse design formulations. This is a difficult strategy because realizable targets are not known in practice. Recent attempts to replace inverse design by direct design optimization attempt to remove the dependence on targets. However, direct optimization has unresolved problems related both to physical modeling and optimization problem formulation; e.g., it is not clear what to optimize. In this presentation, we discuss alternative optimization formulations and their consequences.

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**MS39****Shape Optimization of Axisymmetric Bodies Subject to Aerodynamic Heating and Ablation**

A common approach for mitigating the heat load of bodies subject to strong aerodynamic heating is through the use of ablative coatings. As the surface ablates the shape of the body changes, altering the flow, aerodynamic forces, and heat loads on the body. We present a computational analysis and design optimization framework for aerodynamically heated structures that accounts for this transient nonlinear interaction and the heat transfer through the body using high-fidelity numerical models.

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**MS39****Supersonic Aircraft Design: Challenges for Optimization**

This presentation highlights the application of numerical optimization to several problems in supersonic aircraft design, including the shape optimization of configurations with laminar flow and tailored boom signatures. These problems pose difficulties for conventional gradient-based optimization due to their discontinuous behavior, the need for high fidelity analysis, and the absence of efficiently-generated sensitivity information. The talk will describe some of the techniques used to address these problems, including gradient-free search methods and emerging multi-fidelity modeling strategies.

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**MS39****Multifidelity Optimization Methods for Supersonic Aircraft Design**

Supersonic aircraft design aims to eliminate the efficiency, environmental, and performance barriers to practical supersonic cruise vehicles. The high computational costs of high-fidelity supersonic aircraft simulations motivate methods to significantly reduce the cost of design optimization. One avenue of interest is multifidelity methodology: using multiple models with differing levels of accuracy and computational cost. This work will identify promising approaches for incorporation of multifidelity models in supersonic design.

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**MS40****Optimization in Radiation Therapy**

We give an overview of all aspects of treatment planning, including the large scale optimization problem, which is solved for each individual patient based on the geometry and clinical state of his or her disease. We end with a discussion of multi-objective optimization, a current research topic in radiotherapy which addresses the inherent trade-offs (tumor coverage versus healthy tissue sparing) involved in radiation delivery.

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**MS40****Control Policies for Off-Line Adaptive Radiation Therapy**

Optimization-based planning of radiation treatments often produces sharp dose gradients between tumors and healthy tissue. Due to random shifts during treatment, significant differences between the “optimized” plan and the actual dose can occur. Radiation is delivered as a series of small daily fractions, and we exploit the dynamic nature of treatment and information gathering by adapting the plan to fraction-to-fraction variations measured during a patient’s treatment course within a DP framework and using Bayesian updating.

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**MS40****Optimal Multileaf Collimator Leaf Sequencing in IMRT Treatment Planning**

Optimized intensity profiles should be decomposed into deliverable apertures and corresponding intensities so that total radiation therapy treatment time is minimized. We develop the first exact algorithm capable of solving real-world problem instances to optimality (or to within provably small optimality gaps) within practicable computational limits, using a combination of integer programming decomposition and combinatorial search techniques. We demonstrate the efficacy of our approach on a set of 25 clinical test instances.

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**MS40****Specifying Dose Distribution Requirements for the Robust IMRT Treatment**

Radiation therapy is a dominant modality in treating various cancers. IMRT, its high-precision counterpart, is a state-of-the-art tool for this type of treatment. We investigate the possibility of including the dose distribution prescription (specified by the so-called dose-volume histograms) within the robust IMRT treatment planning framework -the approach that allows to minimize the negative impact of the inherent uncertainties- and relate this question to the classical problem of moments.

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**MS41****Differential-Geometric Foundations of Eigenvalue Algorithms**

The formulation of the extreme symmetric eigenvalue problem as an optimization problem on a nonlinear manifold opens avenues for using several recently proposed differential-geometric optimization methods. We present a general theory of Newton, trust-region, and conjugate-gradient methods on Riemannian manifolds, and we show how these abstract algorithms yield concrete, competitive numerical algorithms for the symmetric eigenvalue problems, some of which shed a new light on the convergence behavior of certain classical algorithms.

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**MS41****An Implicit Riemannian Trust-Region Method**

We propose and analyze an “implicit” trust-region method in the general setting of Riemannian optimization. The method is implicit in that the trust-region is defined as a superlevel set of the  $\rho$  ratio of the actual over predicted decrease in the objective function. This approach replaces the trust-region heuristic with a meaningful performance measure and abandons the classical accept/reject mechanism to improve efficiency. The new method inherits the convergence properties of the generic Riemannian trust-region method. Improved efficiency is demonstrated on the problem of computing extreme eigenspaces of a symmetric definite matrix pencil.

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**MS41****Direct Search Methods Over Manifolds**

We’ll examine how direct search methods can be employed over manifolds. Our main effort will be devoted to developing pullback procedures for the  $C^2$  and  $C^1$  Riemannian manifold cases using geodesics and the implicit function theorem. This allows us to redefine our problem as an equivalent one in some Euclidean space  $R^n$  for an  $n$ -dimensional manifold. Applications to equality constrained problems. We’ll also briefly examine the Lipschitz manifold case.

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**MS41****Higher-Order Tensors: Best Rank Approximation Algorithms**

Higher-order tensors are generalizations of matrices in the same way as matrices are generalizations of vectors. They have various application areas, such as biomedical engineering, image processing, scientific computing, and signal processing. Contrary to the matrix case, the best rank- $(R_1, R_2, \dots, R_N)$  approximation of tensors cannot be obtained in a straightforward way. In this talk, we present the higher-order orthogonal iterations algorithm and derive two new algorithms that solve this problem, based on the trust-region and conjugate gradient methods on manifolds. We touch on some of the applications.

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**MS42****Multilevel Semismooth Newton Methods for Elastic Contact Problems**

We consider the application of semismooth Newton methods to the solution of elastic contact problems. We show that for a regularized problem the convergence is super-linear. Moreover we present an error estimate depending on the regularization parameter. We show that multilevel methods can be applied to solve the semismooth Newton method and prove mesh-independent convergence of the multilevel method. Finally, we present numerical results.

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**MS42****Biofilm Characterization Using Large Scale Optimization**

Biofilms occur in aqueous systems ranging from water distribution networks to human physiology. We use level set methods driven by convection for the interface transport and diffusion-reaction dynamics for the nutrient consumption to predict biomass behavior. An inverse problem is formulated to calibrate initial conditions and reaction coefficients by reconciling the differences of experimental observations and numerical predictions. The implementation uses C++ abstraction concepts to efficiently implement the forward and adjoint equations.

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**MS42****Solving the Trust-Region Subproblem Using Multilevel Techniques**

We propose a new technique to be used along with multilevel methods that solves the trust-region subproblem by applying a multilevel version of the Mor-Sorensen method. The main advantage of this approach is to be able to find second-order solutions to the minimization problem for 3D-

problems and large scale discretizations. We present here the new method, some numerical results and possible future discussions.

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**MS42**  
**Adaptive Multilevel Inexact SQP-Methods for PDE-Constrained Optimization**

We present a class of adaptive multilevel inexact SQP-methods for the solution of optimization problems governed by nonlinear PDEs. Starting with a coarse FE-discretization of the underlying optimization problem we combine an efficient trust-region SQP-method with an implementable adaptive refinement strategy based on estimators. The algorithm uses implementable accuracy requirements for the inexactness in iterative linear equation solves. We prove global convergence to a first-order optimality point of the infinite-dimensional problem. Numerical results are presented.

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**MS43**  
**PDE-Constrained Optimization Problems and the Challenge of Finding Good Preconditioners**

The nature of the quadratic sub-problems within PDE-constrained optimization problems means that iterative methods are frequently used to solve the resulting saddle-point systems. By exploiting the very specific block structure for several classes of such problems, we will show that efficient and effective preconditioners can be formed. The sensitivity of the quality of the preconditioner with respect to the regularization parameter in the problem will also be discussed.

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**MS43**  
**Preconditioned Iterative Methods for Generalized Saddle Point Problems**

We discuss the formulation and analysis of preconditioned iterative methods for the solution of generalized saddle-point problems. We focus on those characteristics of saddle-point problems that are peculiar to interior methods for general nonlinear optimization, such as inertia detection, approximate preconditioning and the treatment of inherent ill-conditioning.

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**MS43**  
**An Overview of Iterative Solvers for Saddle Point Systems**

In this talk I provide an overview of iterative methods for solving saddle point (KKT) linear systems. We focus on preconditioned Krylov subspace iterations with block preconditioners. Issues such as how to exploit the structure of the problem and how to effectively approximate the primal and dual Schur complements are to be discussed. Spectral analysis of preconditioned matrices is provided and widely used preconditioning techniques are described, along with a few numerical examples.

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**MS43**  
**Preconditioners for Semidefinite Programming**

Semidefinite programming has become a valuable paradigm whose practical impact is mainly limited by the ill-conditioned large dense systems of linear equations that arise when implementing primal-dual interior-point methods. We propose preconditioners for solving these systems by iterative methods.

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**MS44****Detection of 16-QAM Signaling in MIMO Channels**

We develop a computationally efficient approximation of the maximum likelihood (ML) detector for 16 quadrature amplitude modulation in multiple-input multiple-output (MIMO) systems. The detector is based on solving a convex relaxation of the ML problem by an affine-scaling cyclic Barzila-Borwein method for box constrained relaxation problem. Simulation results show that this proposed approach outperforms the conventional decorrelator detectors. Moreover, the complexity of the proposed approach is much less than that of other detectors.

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**MS44****An Ellipsoidal Branch and Bound Algorithm for Global Optimization**

A branch and bound algorithm is developed for global optimization. Branching in the algorithm is accomplished by ellipsoidal bisections while bounds are obtained by computing the best linear underestimate for the concave part of the objective function restricted to an ellipsoid. An iterative approach for solving convex relaxations of the original problem is developed which is based on successive ball approximations to the original set. This algorithm is a generalization an earlier scheme of Lin and Han. Numerical experiments are reported.

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**MS44****Multilevel Algorithms For Linear Ordering Problems**

Linear ordering problems appear in many applications of large sparse matrix computation, VLSI design, biological applications, graph drawing, etc. Many heuristic algorithms (e.g., Spectral Sequencing, Optimally Oriented Decomposition Tree, Multilevel based, Simulated Annealing, Genetic Hillclimbing, etc.) were developed in order to achieve near optimal solution. We present a general framework of linear time multilevel heuristic algorithms (MA) especially designed for linear ordering problems. We demonstrate how the building blocks of the general MA can be used in various ways to make it suitable for solving different functionals. We show how the bandwidth of a graph can be approximated by a continuation approach in which a sequence of minimum p-sum solvers are embedded

with progressively larger p.

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**MS44****Quadratic Programming Techniques for Graph Partitioning**

In this talk, we are going to present quadratic programming-based block exchange techniques for graph partitioning. Our numerical experiments indicate these techniques may yield a significant improvement in the partition quality.

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**MS45****CSDP: A Parallel Implementation of a Primal-Dual Method for SDP.**

CSDP is a subroutine library and stand-alone solver for semidefinite programming problems. CSDP is an open source software package that has been published through the COIN-OR repository. This talk will focus on recent improvements and future plans for CSDP including CSDP's use of OpenMP on shared memory parallel systems. Computational results will be presented.

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**MS45****The SDPA Project: Solving Large-Scale Semidefinite Programs**

In 1995, we started the SDPA Project aimed for solving large-scale SDPs with numerical stability and accuracy. The SDPA (SemiDefinite Programming Algorithm) is a C++ implementation of a Mehrotra-type primal-dual predictor-corrector interior-point method for solving the standard form SDP and its dual. In this talk, we show some special features and future plans of the SDPA Project.

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#### MS45

##### Reimplementing SeDuMi: A Progress Report

SeDuMi was a Matlab based solver for optimization over symmetric cones. To overcome various difficulties with Matlab we started to reimplement it using Python in late 2007. In this talk we present our progress about this software challenge.

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#### MS45

##### Computational Experiences in Solving Large-Scale SDP

We report our computational experiences on solving large scale SDPs via a primal-dual interior-point method for which the linear system at each iteration is solved by a preconditioned iterative method. We tested our algorithms on large scale SDPs from relaxation of combinatorial and distance geometry problems, as well as nearest correlation matrix problems in statistics. We also discuss the construction of preconditioners and related computational issues for the linear systems.

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#### MS46

##### A Large-Update Infeasible Interior-Point Algorithm Based on the Logarithmic Barrier Function for Linear Optimization

Recently an  $O(n)$  infeasible full-Newton step interior-point method was presented during which the iterates move in a small neighborhood (the region of quadratical convergence) of the central path of perturbed problems. We in-

roduce a long-step version of the algorithm. So the iterates may temporarily get far from the central path of perturbed problems. Using a few damped centering steps we return them to the central path corresponding to the new value of the barrier parameter.

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#### MS46

##### A New Search Direction for Self-Dual Embedded Semidefinite Optimization

In the literature on interior-point methods for semidefinite optimization, one key point is the need for well defined search directions, with blocks (in the direction) corresponding to symmetric matrices being symmetric. In the talk, a new search direction is proposed; the idea underlying is to force these blocks to be symmetric by using linear constraints. Primary numerical test shows that to some extent our new search direction is comparable with the Nesterov-Todd direction.

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#### MS46

##### Superlinear Convergence of an Infeasible-Interior-Point Method for Linear Optimization

Recently a primal-dual infeasible interior-point algorithm has been proposed for linear optimization that uses only full Newton steps. The iteration bound of this algorithm coincides with the best known bound for infeasible interior-point algorithms. Each iteration of the algorithm consists of a so-called feasibility step and some (usual) centering steps. In this paper we present a slightly different algorithm and we prove that the algorithm is Q-superlinearly convergent, while the complexity is the same as before.

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#### MS46

##### A New Primal-Dual Infeasible Interior-Point Algorithm for Second-Order Cone Optimization

We present a primal-dual infeasible interior-point algorithm for second-order conic optimization. It generalizes a recently published algorithm for linear optimization. It is proven that the number of iterations of the algorithm is bounded by  $O(N \log(N/\epsilon))$ , which coincides with the well-known best iteration bound for such algorithms. Here  $N$



stands for number of second order cones in the problem formulation and  $\varepsilon$  for the desired accuracy.

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#### MS47

##### Set-Semidefinite Optimization and Its Order Structure.

We introduce set-semidefinite optimization as a new field of vector optimization. We study vector-valued optimization problems having an inequality constraint with a special partial order in the space of linear maps. This order considers quadratic forms being non-negative on a set  $K$ . In finite dimensions one obtains for  $K = \mathbf{R}^n$  semidefinite and for  $K = \mathbf{R}_+^n$  copositive optimization problems. For the associated ordering cone calculation rules, characterizations and results on the dual and on the interior are presented.

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#### MS47

##### Set-Valued Duality in Vector and Set Optimization.

We present a duality scheme for set-valued function that is based on a new notion of affine minorants. Concepts like properness, convexity, sublinearity, indicator and support functions, conjugates, inf-convolution and result like biconjugation and Fenchel–Rockafellar duality theorems are established within the new framework. Proofs do not rely on the corresponding scalar theory, but many results can be given an equivalent formulation for a family of scalar problems. We apply the theory to linear vector optimization problems and to set-valued convex risk measures.

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#### MS47

##### An Existence Result for Equilibrium Problems With Some Surjectivity Consequences

We present conditions for existence of solutions of equilibrium problems, which are sufficient in finite dimensional spaces, without making any monotonicity assumption on the bifunction which defines the problem. As a consequence we establish surjectivity of set-valued operators of the form  $T + \lambda I$ , with  $\lambda > 0$ , where  $T$  satisfies a property

weaker than monotonicity, which we call pre-monotonicity. We study next the notion of maximal pre-monotonicity. Finally we adapt our condition for non-convex optimization problems, obtaining as a by-product an alternative proof of Frank-Wolfe's Theorem.

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#### MS47

##### Optimality Conditions, Duality and Penalty Approach in Set-Semidefinite Optimization

Set-semidefinite optimization is a new unified approach in vector optimization covering semidefinite and copositive optimization and optimization with second-order optimality conditions as constraints. For this general problem class we give necessary and sufficient optimality conditions as well as duality results. A penalty approach is presented for the treatment of the special quadratic constraint arising in set-semidefinite optimization.

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#### MS48

##### Newton Methods for Generalized Nash Equilibrium Problems

In the generalized Nash equilibrium problem both the objective function and the feasible set of each player may depend on the other players' strategies. Although this equilibrium problem is an important modeling tool its use is limited by its analytical complexity. We therefore consider several Newton methods, analyze their features and compare their range of applicability. In particular, we address the issue of the non local uniqueness of the solutions that can cause severe difficulties.

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#### MS48

##### On the Numerical Performance of an Interior Point Method for Complementarity Problems

We discuss the numerical performance of a new interior point method for solving linear complementarity problems.

The algorithm uses one matrix factorization and  $m$  back-solves at each iteration. Different factorization subroutines can be chosen in order to take advantage of the structure of the problem. Numerical results are presented for a large collection of linear complementarity problems arising in the simulation of multibody systems with contacts and friction and in equilibrium problems for energy markets.

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**MS48**

**Complementarity Problems over Symmetric Cones**

We present a class of interior point methods for solving linear complementarity problems over symmetric cones. The methods use adaptive long steps to produce iterates in a wide neighborhood of the central path. We prove polynomial complexity, and we give sufficient conditions under which the duality gap converges superlinearly to zero. We also describe two large scale practical applications involving direct products of second order cones and cones of positive semidefinite matrices.

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**MS48**

**Homogeneous Algorithms for Monotone Conic Complementarity Problems**

For monotone conic complementarity problems, a homogeneous model has been proposed for which a bounded path having a trivial starting point exists: if the problem is solvable then it gives us a solution, if the problem is strongly infeasible, then it gives us a certificate proving infeasibility. We describe a class of algorithms for tracing the path above. For linear problems, polynomial iteration complexity bounds of the algorithms are derived.

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**MS49**

**The DAKOTA Toolkit for Parallel Optimization and Uncertainty Analysis**

DAKOTA is a Sandia National Laboratories toolkit for optimization, uncertainty quantification, and sensitivity analysis with large-scale computational models. Through strategies, its algorithms may be combined with each other and/or with global or local surrogate models. I will survey the DAKOTA framework, including available methods, modes of parallelism, and design abstractions. Examples including surrogate-based optimization, optimization under uncertainty, and efficient global reliability assessment will illustrate benefits of hybrid methods. DAKOTA is freely available from <http://www.cs.sandia.gov/DAKOTA>.

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**MS49**

**Computing Architectures for Design Space Exploration Methods**

Over the last few years great progress has been made in design space exploration methods. These methods have in common that they generally address problems involving long running computer codes. They can try to provide an understanding of the relationship between inputs and outputs, perform single- or multi-objective optimizations, or design under uncertainty. To successfully apply these methods appropriate architectures are needed. This talk will provide an overview of such architectures.

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**MS49**

**The Acro/COLIN Framework: Developing Flexible Optimization Interfaces for Parallel, Hybrid, and Dynamically-Configured Algorithms**

Most optimization programming interfaces force both the application and the algorithm to use common data types and common optimization problem models (e.g. MINLP). In contrast, the Acro/COLIN framework decouples data type dependence between application and algorithm, supports extensible problem representations, and facilitates the rapid construction of hybrid algorithms. We will present an overview of the core capabilities of Acro/COLIN and its application to the development of Agent-based Optimization, a hybrid asynchronous optimization meta-algorithm.

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**MS49**

**Manifold-Based Learning and Search Techniques for Semi-Interactive Global Optimization**

Recent experimental evidence indicates high-quality solutions to global optimization problems can reside on low-dimensional non-linear manifolds. The existence of such manifolds has key implications for the design of both automated and semi-interactive global optimization algorithms. We discuss techniques for identifying such manifolds on standard benchmark problems, surrogate search algorithms based on the resulting manifolds, and semi-interactive search driven by human manifold analysis.

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**MS50**

**An Optimization Approach for Generating Se-**

### quences of Radiotherapy Treatment Plans

A method for generating sequences of intensity-modulated radiotherapy treatment plans is presented. The goal is to support the physician in finding a sound trade-off between plan quality and treatment complexity. The method is influenced by column generation approaches and alternates between solving a nonlinear problem and a restricted convex problem. Similarities between the proposed method and the conjugate-gradient method for convex quadratic programming problems are discussed. Results on clinical cases are presented as well.

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### MS50

#### Blending Mathematics, Computation and Physics into a Treatment Planning System

Optimally designing radiotherapy treatments is a popular and meaningful area of research, but the community lacks a complete open-source treatment system that can accommodate head-to-head comparisons of varying techniques. We will discuss the design and implementation of a research oriented treatment design system that begins with a patient's geometry and prescription and ends with a treatment tailored to the treatment paradigm. To facilitate broad testing of individual steps within the process, the system is built in modules that can be substituted with competing techniques.

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### MS50

#### Large-Scale Optimization Strategies for Optimal Cancer Treatment Design

Treatment planning for radiation therapy is inherently complex due to the number of input parameters involved. The complexity is amplified by the uncertainty of target shapes due to organ motion, by dose estimation, by availability of biological information, and by competing multiple clinical objectives within the planning procedure. In this talk, we describe some of our experience in cancer treatment design related to these issues. Various optimization methods will be contrasted, and computational challenges will be discussed. This work is joint with medical researchers from Washington University St. Louis.

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### MS50

#### Optimization of Image Guided Radiation Therapy

Intensity Modulated Radiation Therapy (IMRT) treatments are typically delivered in daily fractions rather than a single session. Recent developments in Image Guided Radiation Therapy (IGRT) are promising to provide dynamic information about the state of the tumor. This presentation discusses optimization models that update the plan after every fraction and achieve the best IMRT design for both fraction and overall treatment with the aim of capturing the changes in tumor position and the shape.

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### MS51

#### Probably Optimal Solutions to Geometric Vision Problems

In the past, the main methods for solving problems in Multiview Vision Geometry have been iterative techniques, which may suffer from falling into local minima, and trouble with convergence. Recent research has turned to finding guaranteed globally optimal solutions to such problems. Techniques include quasi-convex optimization, Second Order Cone Programming, Branch-and-bound techniques and fractional programming, solving many of the common vision geometry problems. In this talk, we address problems such as essential-matrix estimation, many-view triangulation and motion of a vehicle with rigidly placed cameras. We provide optimal solutions, (in L2 or L-infinity norm) where no such solution existed previously (as of 2007).

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### MS51

#### Invariance Properties of Newton-Type Methods on Reductive Homogeneous Spaces

Newton-type methods on differentiable manifolds became recently very popular, from a theoretical and from an application point of view as well. We discuss invariance properties for these methods on a very rich class of smooth manifolds, namely reductive homogeneous spaces. The invariance properties we present are a generalisation of the well known affine invariance properties of Newton's method on Euclidean spaces. A few examples from signal processing and computer vision are given to explain the details.

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**MS51****Local Convergence Properties of Conjugate Gradient Methods on Manifolds**

The local convergence properties of conjugate gradient methods on smooth manifolds are usually harder to analyse than their counterpart on vector spaces. We present recent results in this direction, exemplified by implementations of the CG method in the area of signal processing, namely simultaneous diagonalisation of several covariance matrices.

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**MS51****The Basis Partition of the Space of Linear Programs**

We consider the space of all linear programs with  $n$  non-negative variables and  $m$  equality constraints. Each linear program (LP) is associated with a basis (a basis is a subset of indices  $1, 2, \dots, n$ ), in the sense that the limit of the central path of the LP, which is an optimal solution of the LP, corresponds to a unique basis. There are only a finite number of bases. Thus, the space of linear programs (SLP) can be partitioned into a finite number of sets  $S_1, S_2, \dots, S_k$ , each set containing all LPs which are associated with a common basis, (so called the basis partition). If this partition of the SLP can be explicitly characterized, then we can solve any set of (infinitely many) linear programs, e.g. a parametric LP, in the closed form. A novel tool for characterizing this partition of the SLP is presented as follows. Relating to the central path, there exists a universal ordinary differential equation  $M' = h(M)$  defined on projection matrices  $M$ . For any LP, one can define a projection matrix, starting from which the solution of  $M' = h(M)$  converges to a limit projection matrix which can determine the optimal basis of the LP. This establishes a corresponding partition on the space of projection matrices, denoted by  $G$ .  $G$  is the well-known Grassmann manifold. With the help of the vector field  $h(M)$  on the Grassmann manifold  $G$ , it is promising to discover full characterization of the partition of the SLP. We will present some properties related to the SLP found so far. Full structure of the basis partition of SLP is still awaiting an exploration.

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**MS52****Multi-Secant Equations, Approximate Invariant Subspaces and Multigrid Optimization**

New approximate secant equations are shown to result from

the knowledge of (problem dependent) invariant subspace information, which in turn suggests improvements in quasi-Newton methods for unconstrained minimization. It is also shown that this type of information may often be extracted from the multigrid structure of discretized infinite dimensional problems. A new limited-memory BFGS using approximate secant equations is then derived and its encouraging behaviour illustrated on a small collection of multilevel optimization examples. The smoothing properties of this algorithm are considered next, and automatic generation of approximate eigenvalue information demonstrated. The use of this information for improving algorithmic performance is finally investigated on the same multilevel examples.

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**MS52****Control Constrained Optimal Control of Time-Dependent Convection Diffusion by the Discontinuous Galerkin Method  $dg(1)$  in Time and SDFE(streamline Diffusion Finite Element) Discretization in Space**

We consider optimal control of (time-dependent) convection diffusion equations. To discretize the optimal control problem we use the variational discrete concept proposed in [?]. In this approach the cost functional is approximated by a sequence of functionals which are obtained by discretizing the state equation with the help of a  $dg(1)$  discretization in time and SDFE discretization in space. The control variable is not discretized. Error bounds for control and state are obtained both in two and three space dimensions. The numerical implementation of a semi-smooth Newton method for the variational-discretized problem is described in detail. Finally, we present numerical experiments which confirm our analytical findings.

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**MS52****A Multilevel Adaptive Cubic Overestimation Technique**

C. Cartis, N. Gould and Ph. Toint have recently proposed a new algorithm for unconstrained nonlinear optimization where a cubic model of the objective function is constructed at each iteration. The model cubic term is then updated using a "trust-region radius update"-like process. In this talk, we present the application of the multilevel philosophy to this method, some numerical results and possible future discussions.

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**MS52****Multilevel Trust-Region Methods for Bound-Constrained Optimization**

We present a globally convergent multilevel trust-region method for large-scale bound-constrained optimization problems. The method relies on a coarse-to-fine hierarchy of objective functions. This setting arises, e.g., when infinite-dimensional optimization problems are discretized at different scales. The algorithm uses the coarser versions to generate steps in a way similar to the full approximation multigrid scheme. The bound constraints are handled by an active-set strategy and by a natural feasibility condition on lower levels.

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**MS53****Uncertainty Quantification in PDE-Based Inverse Problems**

The structure of many PDE-based inverse problems permits very fast solution and very cheap approximation of the Hessian of the misfit via inexact Newton-CG methods (where "fast" and "cheap" mean at a cost of a constant number of forward solutions). The connection for the linear/Gaussian case between minimization of regularized least squares misfit functions and full Bayesian inverse solution underscores the role of fast optimization methods in uncertainty quantification. We discuss some preliminary ideas on how such structure-exploiting techniques can be brought to bear on Bayesian analysis of nonlinear/non-Gaussian inverse problems. Examples from state estimation for advective-diffusive transport and parameter estimation for wave propagation are used to illustrate the main ideas.

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**MS53****Optimal Control of the Thermistor Problem**

The presented talk deals with the optimal control of the thermistor problem that models the conductive heat transfer in a conductor produced by an electric current. This leads to a quasi-linear system of partial differential equations (PDEs) with mixed boundary conditions. A possible application for this coupled system of PDEs is the hardening of steel workpieces via the Joule effect. However, for practical applications, it is necessary to obey pointwise state constraints that guarantee that the melting temperature is not exceeded. This kind of constraints is known to be numerically and theoretically challenging to handle since continuity of the state is required and the associated multipliers are only measures in general. Using maximum parabolic and elliptic regularity results, we establish continuity of the state and existence for solutions of the adjoint equation which leads to first-order necessary conditions. The problem is solved numerically by means of a Moreau-Yosida type regularization of the state constraints. The feasibility of this approach is afterwards demonstrated by the example of hardening a gear rack.

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**MS53****On an ODE-PDE Constrained Optimal Control Problem with Applications to Hypersonic Flight Under Heat Load Constraints**

During ascent and reentry of a hypersonic space vehicle into the atmosphere of any heavenly body, the space vehicle is subjected to extreme aerothermic loads. Therefore an efficient, sophisticated and lightweight thermal protection system is determinative for the success of the entire mission. For a deeper understanding of the conductive, convective and radiative heating effects through a thermal protection system, a mathematical model is investigated which is given by an optimal control problem subject to not only the usual dynamic equations of motion and suitable control and state variable inequality constraints for the ODE part of the problem, but also subject to an instationary quasi-linear heat equation with nonlinear boundary conditions and a state constraint, forming the PDE part of the problem. By this model the temperature of the heat shield can be limited in certain critical regions. The resulting ODE-PDE constrained optimal control problem is, because of its complexity, solved by the approach *First discretize, then optimize*. The discretization scheme used is a second-order finite-volume scheme in space for the semi-discretization of the quasi-linear parabolic partial differential equation in its space variables. This yields a large scale nonlinear ODE constrained optimal control problem with multiple state

and/or control variable inequality constraints, in particular for the limitation of the heat load. This problem is also solved by the approach *First discretize, then optimize* and ends in a large scale non-linear programming problem. Numerical results are presented. They show, that the aerothermic load and the fuel loss can be considerably reduced by optimization. Some theoretical light on this problem is given by the investigation of an academic problem of an equivalent structure, which is based on the well-known classical harmonic oscillator problem, which has illustrated the development of the maximum principle and therefore is called the hypersonic oscillator.

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### MS53 Optimization Methods for Some Problems in Finance

In this talk we consider several aspects of optimization problems in finance from a numerical point of view. In particular we investigate the use of optimization methods for calibration problems and their relation to nonlinear least squares problems. These problems are formulated as PDE-constrained optimization problems as well as optimization problems with SDE-constraints. We discuss the numerical solution and the use of adjoint variables in this context. We apply these techniques to some calibration problems for standard and nonstandard models for the pricing of options.

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### MS54 Obtaining Optimal k-Cardinality Trees Fast

Given an undirected graph  $G = (V, E)$  with edge weights and a positive integer number  $k$ , the  $k$ -Cardinality Tree problem is to find a subtree  $T$  of  $G$  with exactly  $k$  edges and the minimum possible weight. Many algorithms have been proposed to solve this NP-hard problem, resulting in mainly heuristic and metaheuristic approaches. In this paper we present an exact ILP-based algorithm using directed cuts. We mathematically compare the strength of our formulation to the previously known ILP formulations of this problem, and give an extensive study on the algorithm's practical performance compared to the state-of-the-art metaheuristics. In contrast to the widespread assumption that such a problem cannot be efficiently tackled by exact algorithms for medium and large graphs (between 200 and 5000 nodes), our results show that our algorithm not only has the advantage of proving the optimality of the computed solution, but also often outperforms the meta-

heuristic approaches in terms of running time.

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### MS54 Strong Formulations for 2-Node-Connected Steiner Network Problems

We consider a survivable network design problem known as the 2-Node-Connected Steiner Network Problem (2NCON): we are given a weighted undirected graph with a node partition into two sets of customer nodes and one set of Steiner nodes. We ask for the minimum weight connected subgraph containing all customer nodes, in which the nodes of the second customer set are nodewise 2-connected. This problem class has received lively attention in the past, especially with regard to exact ILP formulations and their polyhedral properties. In this talk, we present a transformation of this problem into a related problem considering directed graphs and use this to establish two novel ILP formulations to solve 2NCON, based on multi-commodity flow and on directed cuts, respectively. We prove the advantages of our formulations and compare both approaches theoretically as well as experimentally. Thereby we solve instances with up to 1600 nodes to provable optimality.

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### MS54 Multi-Period Traffic Routing in Satellite Networks

We introduce a traffic routing problem over an extended planning horizon that appears in geosynchronous satellite networks. Unlike terrestrial networks, routing on a satellite network is not transparent to the customers. As a result, a route change is associated with significant monetary penalties that are usually in the form of discounts (up to 40%) offered by the satellite provider to the customer that is affected. The notion of these re-routing penalties requires the network planners to look at routing decisions over multiple time periods and introduces novel challenges

that have not been considered previously in the literature. We develop a branch-and-price-and-cut procedure to solve both the deterministic and stochastic version of this problem and describe an algorithm for the associated pricing problem. Computational work will be discussed.

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#### MS54 Approaches for a Single-Source Network Design Problem

Let us consider a network  $G=(N,A)$  where a node is a source and some others are destinations. Each arc is related to a set of cables, and these cables are sorted in types according to capacities. A cable type can only be used for an arc if all the precedence types have also been used for this arc. The problem is to decide the cables to install in each arc to guarantee serving the demands of all destinations from the source at minimum cost. We analyze and compare different flow formulations and their flow-projected formulations. We also discuss the variant where the solution must be a tree.

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#### MS55 New Worst Cases for Polynomial Optimization Via Group-Invariant SDPs

This talk presents the first unrestricted family of polynomials which are non-negative but not sums-of squares. The presented construction demonstrates the use of group-representation theory in semi-definite programs (SDP) resulting from polynomial optimization problems. Surprising at first sight only, not every non-negative (PSD) polynomial is a sum of squares (SOS) of other polynomials. The relation between PSD and SOS polynomials is far from being only a historically challenging topic; the hardness of polynomial optimization actually comes in via the difference between the two. But although there are (provably) many polynomials which are PSD but not SOS, few are currently known. The talk presents a family of PSD polynomials which are not SOS, encompassing all previously known examples. Moreover, the construction presented in the talk may serve as an explicit example of the use of

group-representation theory in order to reduce the size of SDPs.

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#### MS55 Properties of Symmetry Reduction for Semidefinite Programs

In this talk we consider the mathematical properties of certain symmetry reductions for semidefinite programs (SDP's), where the SDP data matrices lie in some matrix algebra. We generalize the so-called regular \*-reduction technique to this setting, and provide some examples to illustrate the procedure. We also compare various other reduction techniques from the recent literature to the regular \*-reduction.

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#### MS55 Exploiting Group Symmetry in SDP Relaxation of the QAP

The Quadratic Assignment Problem (QAP) contains the traveling salesman problem as a special case and even small instances are notoriously difficult to solve in practice. In this talk we consider semidefinite programming relaxations of the QAP, and show how to exploit algebraic symmetry of the data matrices when present, in order to greatly reduce the size of the relaxations. This approach has allowed us to compute the best known bounds for several instances from QAPLIB.

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#### MS55 Lower Bounds for Measurable Chromatic Numbers

The chromatic number of  $n$ -dimensional Euclidean space is the minimum number of colors needed to color all points so that no two at unit distance get the same color. One speaks of the measurable chromatic number when the color classes are measurable. Finding the (measurable) chromatic number of the plane is a famous open problem. Using a generalization of Lovasz theta-function and basic tools from functional analysis we obtain new lower bounds in several dimensions.

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### MS56

#### **YAS: An Open-source C++ Platform for Rapid IPM Development with SMP**

We present an object-oriented open-source platform YAS (Yet Another Solver) for rapid porting, prototyping and development of interior-point method algorithms in C++, targeted for SMP architecture – symmetric multiprocessing with multiple CPUs sharing a common memory. YAS is particularly designed to allow easy extensions of IPM beyond the symmetric cone programming, e.g.,  $p$ -norm cones, and the underlying direct linear algebra solvers, e.g., PCG. To achieve near-peak CPU performance, YAS provides a transparent interface between pre-tuned BLAS libraries, such as Intel MKL, AMD ACML and ATLAS. To take the advantage of some common features of IPM and the linear algebra, special objects are introduced. Currently within the platform, basic primal short-step, long-step, predictor-corrector, and Nesterovs asymmetric primal-dual predictor-corrector methods are implemented. YAS provides SeDuMi-like data input interface for MATLAB and Octave, with the capability of building standalone applications. In addition, for SDP YAS allows specification of matrix-pencils in their native form.

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### MS56

#### **Criss-Cross Algorithm for General Linear Complementarity Problem**

Fukuda and Terlaky (1992) worked out some connections between Linear Complementarity Problems (LCP) and Oriented Matroids. In their paper they introduced dual problem and proved a Farkas-type alternative theorem. Up to our best knowledge, this is the first paper in which alternative theorem for LCP has been stated and proved. (Their result was called duality theorem by them; however we feel that the alternative theorem for LCP is better name for their result.) Den Hertog, Roos and Terlaky (1993) proved that the minimal index criss-cross algorithm for Linear Complementarity Problem (LCP) is finite if the matrix of the problem is sufficient. Fukuda, Namiki and Tamura (1998) applying the concept of EP-theorem introduced by Cameron and Edmonds (1990) for the LCP problems given by rational data, modified the minimal index criss-cross algorithm in such a way that they either solve the primal LCP, or the dual LCP or give a polynomial size certificate that the matrix is not sufficient. In this talk we show that the minimal index rule can be replaced by the last-in-first-out (LIFO) and most-often-selected-variable (MOSV) rules and still to prove the finiteness of the criss-cross algorithm. Similar modifications that Fukuda, Namiki and

Tamura used in their paper, enables us to generalize our finite variants of the criss-cross method for general LCP problems and to solve those in the sense of the corresponding EP-theorem. Technically, we need to assign label to each variable and update the vector formed from the labels according to the pivot rule. The vector formed from the labels play an important role in proving the finiteness of the criss-cross algorithm. Further generalization of the behaviour of these pivot rules (minimal index, LIFO, MOSV) led to the definition of the class of s-monotone pivot rules and the related results.

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### MS56

#### **Interior Point Algorithms for General Linear Complementarity Problems**

The LCPs are usually NP-hard problems. The largest matrix class where the interior point algorithms (IPM) are polynomial is the class of  $\mathcal{P}_*(\kappa)$ -matrices. We modify the IPMs such that either solve LCPs or give a certificate that proves the matrix does not belong into the class of  $\mathcal{P}_*(\kappa)$ -matrices, or show the unsolvability of the LCP. The modified algorithm is still polynomial, but does not give in all cases a solution for solvable LCPs.

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### MS56

#### **Improved Approximation Bound for Quadratic Optimization Problems with Orthogonality Constraints**

In this talk we consider approximation algorithms for a class of quadratic optimization problems that contain orthogonality constraints, i.e. constraints of the form  $X^T X = I$ , where  $X \in \mathbf{R}^{m \times n}$  is the optimization variable. Such class of problems, which we denote by (QP-OC), is quite general and captures several well-studied problems in the literature as special cases. In a recent work, Nemirovski [Math. Prog. 109:283-317, 2007] gave the first non-trivial

approximation algorithm for (QP-OC). His algorithm is based on semidefinite programming and has an approximation guarantee of  $O((m+n)^{1/3})$ . We improve upon this result by providing the first logarithmic approximation guar-



antee for (QP-OC). Specifically, we show that (QP-OC) can be approximated to within a factor of  $O(\ln \max m, n)$ . The main technical tool used in the analysis is a concentration inequality for the spectral norm of a sum of certain random matrices, which we develop using tools from functional analysis. Such inequality also has ramifications in the design of so-called safe tractable approximations of chance constrained optimization problems. In particular, we use it to improve a recent result of Ben-Tal and Nemirovski [Manuscript, 2007] on certain chance constrained linear matrix inequality systems.

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### MS57

#### Approximate Solutions in Vector Optimization

In vector optimization there are different kinds of approximate solutions. Thus, in the literature we can find Loridan-Kutateladze approximate solutions [2,3], Tanaka approximate solutions [4] and Bonnel approximate solutions [1]. It will be shown that in general these concepts are not equivalent. However, under some suitable hypothesis, we will present some connections between the asymptotical behaviour of sequences of such approximate solutions. References [1] S.Bolintineanu (H.Bonnel), Vector variational principles; "epsilon-efficiency and scalar stationarity," J. Convex Anal., Vol. 8, pp. 71-85, 2001. [2] S.S.Kutateladze, Convex epsilon-programming," Sov.Math.Dokl., Vol. 20, pp. 391-393, 1979. [3] P. Loridan, "epsilon-Solutions in vector minimization problems," J. Optim Theory Appl., Vol. 43, pp. 265-276, 1984. [4] T.Tanaka, A new approach to approximation of solutions in vector optimization problems," in M. Fushini, K. Tone (eds.) Proceedings of APORS 1994, pp. 497-504, World Scientific, Singapore, 1995.

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### MS57

#### A Set-Valued Approach to Duality in Vector Optimization and Applications.

We show that the theory of Multiple Objective Programming (MOP) can be described quite analogously to Single Objective Programming, when it is considered in a set-valued framework. This approach leads to a new duality theory for MOP. For the linear case we present an interpretation of the duality theory which is closely related to the classical idea of "duality of polytopes". As an application we present an algorithm for solving linear multiple objective problems.

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### MS57

#### Multicriteria Optimization in Medical Engineering

Multicriteria optimization problems often arise in medical engineering research. We investigate two nonlinear problems from magnetic resonance imaging (MRI) and particle therapy. In case of MRI, homogeneity of the B1-field and patient exposure were optimized simultaneously with a very large number of constraints, whereas for particle therapy we had several highly nonlinear criteria on ion optics. These problems were solved with a constraint method. We show their special challenges and present numerical results.

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### MS57

#### Lipschitz Properties of the Scalarization Function and Applications.

The scalarization functions were used in vector optimization for a long period. Similar functions were introduced and used in economics under the name of shortage function or in mathematical finance under the name of (convex or coherent) measures of risk. The main aim of this talk is to study Lipschitz continuity properties of such functions and to give some applications for deriving necessary optimality conditions for vector optimization problems using the Mordukhovich subdifferential.

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### MS58

#### Large Scale Cone Complementarity Problems for Rigid Body Dynamics with Contact and Friction

We present a class of iterative methods to solve the cone complementarity subproblems that appear in the simulation of nonsmooth rigid body dynamics with contact and friction. We prove that the method is globally convergent. Through numerical experiments, we demonstrate that the method scales linearly with with an increasing size of the problem up to millions of variables and show that it is very competitive for the simulation of granular flow dynamics.

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### MS58

#### Adjoint Sensitivity Analysis of Hybrid Dis-

**crete/Continuous Systems**

We present a general framework for adjoint sensitivity analysis of a broad class of hybrid discrete/continuous systems described, in their continuous regime, by differential algebraic equation (DAE) systems. This works extend existing results on forward sensitivity analysis of such systems by: (a) considering Hessenberg index-2 DAEs, besides ODE and index-1 DAEs' (b) including the analysis of systems with "memory", that is systems whose dynamics depend on the states (and possibly the state derivatives) at the last transition time, where a discrete event occurred; and (c) providing the analysis for adjoint sensitivity analysis, including the derivation of the appropriate adjoint systems, the equations for the transfer of adjoint variables at transition points, and the resulting sensitivity of the quantity of interest. We provide several illustrative examples, including a more complex model from structural dynamics which uses a hybrid plasticity constitutive material law.

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**MS58****An Algorithm for Finding Equilibria of Stochastic Games**

The talk discusses a hybrid algorithm for finding Nash equilibria of stochastic games. The algorithm combines projected dynamical systems with an interior point method for solving MPEC's. Global convergence results and numerical results will be discussed.

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**MS58****Uniqueness of Solutions for Differential Variational Inequalities**

Differential variational inequalities are differential equations where the right-hand side is determined (in part) by the solutions of variational inequalities. Here we consider linear differential equations with a variational inequality of the form

$$\begin{aligned} \frac{dx}{dt}(t) &= Ax + Bu(t), & x(t_0) &= x_0, \\ u(t) &\in K & \text{for all } t, \\ 0 &\leq (w - u(t))^T(Cx(t) + g(t)) & \text{for all } t. \end{aligned}$$

It has recently been shown that solutions exist if  $CB$  is positive definite, but uniqueness has only be shown in general if  $CB$  is also *symmetric*. Examples of non-uniqueness are demonstrated, and examples of non-symmetric  $CB$  giving uniqueness are shown. Open questions regarding uniqueness are mentioned along with applications of this result.

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**MS59****Recent Numerical Experiences With Large Scale Groundwater Management**

Groundwater management models couple complex groundwater simulation models with optimization techniques. Groundwater simulation models with large spatial domains and long time horizons can present special challenges for successful optimization, even when groundwater flow is the only state under consideration. In this talk, a number of case studies are reviewed highlighting numerical and algorithmic issues that arise in solving large scale groundwater management problems.

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**MS59****Derivative-Free Benchmarking Problems from Water Resources Management**

We present a set of problems from hydrology used to compare derivative-free optimization algorithms. We describe the applications, various simulation-based problem formulations, and show comparison results obtained with a variety of methods including implicit filtering, several implementations of pattern search, a genetic algorithm, DIRECT, and surrogate model approaches. Finally, we provide information about downloading the test problems for the application, testing, and comparison of other applicable optimization algorithms.

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**MS59****A Modified Simulated Annealing Approach for Solving Constrained Optimal Groundwater**

Determining an optimal pump and treat groundwater remediation design subject to constraints defined by maximal concentrations of contamination requires finding the solution to a linear optimization problem bounded by nonlinear constraints. Because parameters defining the properties of groundwater flow are uncertain, a multiscenario approach is taken to include the uncertainty in the model design. When this is done, the objective function, as well as the constraints, are nonlinear and finding a solution to this optimization problem requires the use of an efficient algorithm that avoids unnecessarily calling the flow and transport numerical model. By combining features of a simulated annealing algorithm with a gradient method, a solution to this optimization problem is determined. The method that is presented in this talk is one that dynamically changes as the search algorithm moves through the feasible region, thereby taking into consideration elements such as the approximate gradient of the objective function

and the proximity to the boundary of the feasible region.

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#### MS59

##### POD Calibration for Groundwater Models in ADH

We are solving inverse problems in groundwater modeling. Given values of hydraulic head at discrete locations, we seek to approximate values of hydraulic conductivity for the entire field. We are using ADH, a finite element code developed at the Coastal and Hydraulics Lab in Vicksburg, MS. When using ADH to model large, complex groundwater behavior – for instance the entire state of Florida – extreme run-times prohibit the frequent function calls needed for parameter estimation. Proper Orthogonal Decomposition (POD) is a method to reduce the size of the problem to calibrate ADH, reducing the number of full function calls needed. We will introduce the problem, discuss POD and how it is used for steady-state problems, and demonstrate the accuracy of the POD solution compared to the full ADH solution.

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#### MS60

##### On Solving the Newton Equation System Within Interior-Point Methods for Linear and Conic Optimization Problems.

The purpose of this talk is to review the methods employed to solve the Newton equation system arising within interior-point methods for linear and conic optimization problems. The focus will be on the methods employed in commercial software such as MOSEK. Finally, we will present computational statistics detailing where time is spent when solving the Newton equation system. Moreover, we hope to comment on whether indirect methods such as conjugate-gradient-based methods could be more efficient than direct methods for solving the Newton equation system.

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#### MS60

##### Large-Scale Eigenvalue Problems, Trust Regions and Regularization

We consider large eigenvalue problems for matrices of the form

$$B = \begin{pmatrix} \alpha & g^T \\ g & H \end{pmatrix}$$

where  $H$  is an  $n \times n$  real symmetric matrix,  $g$  is an  $n \times 1$  real vector, and  $\alpha$  is a scalar. Such problems arise, for example, in the context of methods for trust-region subproblems and regularization. We describe the eigenvalue

problem, discuss its connection with the underlying optimization problem, and compare matrix-free approaches such as the Implicitly Restarted Lanczos and the Jacobi-Davidson Methods on large trust-region and regularization problems.

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#### MS60

##### Methods for Large-Scale Eigenvalue Problems in Optimization

We review computational methods for large-scale eigenvalue problems and offer suggestions for some problems of this type arising in optimization.

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#### MS60

##### IDR(s): A New Family of Efficient Algorithms for Large Nonsymmetric Linear Systems

We present a new family of limited-memory iterative methods for solving nonsymmetric systems of linear equations. Our technique is a generalisation of the IDR algorithm of Sonneveld. We describe the methods and illustrate their performance on test problems from applications including interior point methods in optimisation. Our results show that our technique frequently outperforms state-of-the-art Krylov methods such as Bi-CGSTAB and CGS.

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#### MS61

##### Interior-Point Methods for Mixed-Integer Nonlinear Conic Programming

In this talk, we will present a unified framework for solving problems involving nonlinear functions, cone constraints, and discrete variables using an interior-point method. We will give particular consideration to warmstarts and infeasibility identification and present numerical results.

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#### MS61

##### Global Convergence of a Primal-Dual Interior-

### Point Method for Nonlinear Programming

Many recent convergence results obtained for primal-dual interior-point methods for NLP use assumptions of the boundedness of generated iterates. In this talk we discuss how such assumptions can be replaced by new assumptions on the NLP problem and analyze convergence of the new method from any initial guess.

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### MS61

#### Extinguishing Poisson's Spot with Linear Programming

A leading design concept for NASA's upcoming planet-finding space telescope involves placing an occulter 70,000 km in front of a 4-m telescope. The purpose of the occulter is to block the bright starlight thereby enabling the telescope to take pictures of planets orbiting the blocked star. Unfortunately, diffraction effects prevent a simple circular occulter from providing a fully dark shadow—a specially shaped occulter is required. In this talk I will explain how this shape-optimization problem can be solved with linear programming.

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### MS62

#### Multigrid Optimization Schemes for Optimization Problems with Bilinear Structure

Bilinear control problems as distributed parameter estimation problems pose theoretical and computational challenges that are open or have been only partially addressed. We discuss and compare two multigrid-based solution strategies for bilinear optimization problems with bilinear structure. On the one hand, we use the experience gathered with the one-shot multigrid solution to design a collective smoothing multigrid scheme (CSMG). This ap-

proach is quite robust and it provides typical multigrid efficiency. However, its development involves to exploit the specific structure of the problem at hand. On the other hand, we discuss the inherent optimization and globalization properties of the multigrid optimization method (MGOPT) where the multigrid solution framework defines the outer loop of classical optimization schemes. This approach can be successfully applied to problems with very different structure.

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### MS62

#### Multilevel Methods for Constrained Image Registration

In this work we present a new and general framework for image registration when having additional constraints on the transformation. We demonstrate that registration without constraints leads to arbitrary results depending on the regularization and in particular produces non-physical deformations. Having additional constraints based on the images introduces prior knowledge and contributes to reliability and uniqueness of the registration. In particular we consider optimization techniques for the recently proposed locally rigid transformations. In contrast to existing approaches, we propose a constraint optimization framework and do not rely on penalty methods that do not guarantee feasible solutions.

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### MS62

#### Automatically Assessing the Performance of An Optimization-Based Multigrid Method

Many large nonlinear optimization problems are based upon discretizations of underlying continuous functions. Optimization-based multigrid methods are designed to solve such discretized problems efficiently by taking explicit advantage of the family of discretizations. The methods are generalizations of more traditional multigrid methods for solving PDEs. We discuss techniques whereby the multigrid method can assess its own performance, with the goal of automatically determining whether the optimization model is well suited for the multigrid-type algorithm.

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**MS62****A Line Search Multigrid Method for Large-Scale Nonconvex Optimization**

We present a line search multigrid method based on Nash's MG/OPT multilevel approach for solving discretized versions of general unconstrained infinite dimensional optimization problems. Introducing a new condition to a backtracking line search procedure, the step generated from the coarser levels is guaranteed to be a descent direction. Global convergence is proved under fairly minimal requirements on the minimization method used at all grid levels. In particular, our proof does not require that these minimizations, or so-called "smoothing" steps, which we interpret in the context of optimization, be taken at each grid level in contrast with multigrid algorithms for PDEs, which fail to converge without such steps. Preliminary numerical experiments show that our method is promising.

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**MS63****Optimizing Control of SMB Processes with Endpoint Constraints**

Endpoint constraints in the form of terminal sets are a necessary ingredient for guaranteed stability of moving horizon optimizing control strategies. We describe an application of this concept to Simulated Moving Bed Processes. In addition to minimizing a cost function over the prediction horizon, the terminal state is driven to a shrinking set around the optimal steady state operating point. The required product purity is imposed as a constraint in the optimization.

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**MS63****Free Boundary Control in a Viscous Flow Problem**

Considering a viscous inertial Newtonian fluid in an open container, the goal of this work is to move the container off the stand over a certain distance in a given time while keeping the surface smooth and avoiding overflow. The transport of the fluid in the open container is modelled by a free boundary value problem in terms of incompressible Navier-Stokes equations in moving coordinates with no-slip conditions at the walls and kinematic and dynamic boundary conditions at the free surface. The formulation

of the free boundary as graph enables its access to the state variables. Thus, we end up with an pde-constraint optimization problem for the free surface, fluid velocity and pressure – while the outer transport speed acts as control – for which numerical results are presented.

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**MS63****Recent Advances in Optimal Dopant Profiling for Semiconductor Devices**

We present some recent advances for optimal dopant profiling of semiconductor devices. Especially, we discuss the convergence of a generalized Gummel algorithm and show a new approach to solve multi-objective optimal design questions. Both techniques can be easily implemented into existing semiconductor device simulation tools.

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**MS63****Parameter Estimation in Calcium Signaling to the Nucleus of Neurons**

Signal processing in neurons takes place on different levels. For one, electrical signals are propagated in the dendritic tree, towards or away from the soma. Secondly, electrical information that reaches the soma is partially recoded as a calcium wave that propagates towards and into the cell nucleus, activating biochemical reactions which result in the expression of certain genes. To address both signal processing in the dendritic tree of the neuron and calcium signaling at the cell nucleus, we have developed three dimensional volume models based on reconstructed 3-D geometries of neurons and of neuron cell nuclei on which PDEs describe the underlying signaling processes. Embedded in these equations are a number of parameters, such as neuronal membrane capacitance, inner- and outer-neuronal capacitance or diffusion parameters for nuclear calcium. Based on a full 3-D model and experimental data, e.g. recorded from laser-assisted calcium uncaging experiments, inverse models are being developed in order to estimate key parameters in the underlying PDEs. Here we make use of Newton-like and SQP methods which are implemented in our simulation environment UG.

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**MS64****An Open Source Exact Solver for Mixed Integer Non-Linear Programming Problems**

We discuss a spatial branch-and-bound algorithm for non-convex MINLP problems, based on a reformulation tech-

nique for factorable programs. The reformulation library is implemented as a cut generator and is available within the Coin-OR framework ([www.coin-or.org](http://www.coin-or.org)). We present the features of our approach, such as novel branching rules and bound tightening techniques, and show computational tests on instance libraries such as GlobalLib and MinlpLib, and on other instances from industrial applications.

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#### MS64

##### **Primal Heuristics of the Branch-Cut-and-Price-Framework SCIP**

In modern MIP-solvers like the state-of-the-art open source branch-cut-and-price framework SCIP, primal heuristics play a major role in finding and improving feasible solutions at the early steps of the solution process. We give an overview about different categories of heuristics, present a new large neighborhood search heuristic and an improved version of the feasibility pump.

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#### MS64

##### **MIQCP: In Between QCP and MILP**

A natural approach for solving Mixed Integer Quadratically Constrained Programs (MIQCP) is to solve a Quadratically Constrained Program (QCP) at each node in the tree. An alternative is to solve them as MILP using branch and cut. In this talk we will describe and

compare both approaches which are now implemented in ILOG CPLEX.

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#### MS64

##### **State-of-the-Art in Linear and Nonlinear MIP**

Abstract not available at time of publication.

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#### MS65

##### **The Difference Between 5x5 Doubly Nonnegative and Completely Positive Matrices**

The convex cone of  $n \times n$  completely positive (CPP) matrices and its dual cone of copositive matrices arise in several areas of applied mathematics, including optimization. Every CPP matrix is doubly nonnegative (DNN), i.e., positive semidefinite and component-wise nonnegative. Moreover for  $n \leq 4$ , every DNN matrix is CPP. We investigate the difference between  $5 \times 5$  DNN and CPP matrices. We give a precise characterization of how a  $5 \times 5$  DNN matrix that is *not* CPP differs from a DNN matrix, and use this characterization to show how to separate an extreme DNN matrix that is not CPP from the cone of CPP matrices.

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#### MS65

##### **On the Copositive Representation of Binary and Continuous Nonconvex Quadratic Programs**

A recent line of research has shown that a small collection of NP-hard quadratic optimization problems can be represented as linear programs over a specific convex set (the cone of completely positive matrices). Although such convex programs are necessarily NP-hard, their structure allows them to be approximated in a mechanical way up to any accuracy by linear and semidefinite programs. We review these results and then, in the main portion of the talk, show that any nonconvex quadratic program having a mix of binary and continuous variables (for example, all 0-1 integer programs) can be represented in the above fashion. This can be viewed as a broad extension of the aforemen-

tioned earlier results.

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### MS65 An Adaptive Algorithm for Copositive Programs

We consider linear programs over the cone of copositive matrices which arise in integer and nonconvex quadratic programming. We introduce copositivity conditions which we use to define polyhedral inner and outer approximations of the copositive cone. From these, we derive an adaptive linear approximation algorithm for copositive problems. In contrast to previous approaches, our approximation is not uniform but adaptively guided by the objective function. Numerical experience with the algorithm is presented.

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### MS65 Semidefinite and Linear Relaxation Schemes for the Copositive Cone

We propose various semidefinite and linear programming relaxations of the copositive cone. We then examine the tradeoffs in the quality of the relaxations and their computational cost. We rely on the copositive formulation of the stability number of a graph as a benchmark for assessing the quality of the different relaxations.

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### MS66 Probabilistic Analysis of LP

We give an overview of the literature on the probabilistic analysis of linear programming from the early 1980-ies to the present, and we discuss the explanatory power of these results and desirable extensions thereof.

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### MS66 Recent Progress in Primal-Dual Methods for Con-

### vex Optimization

I will review some of the new developments in the theory of primal-dual interior-point algorithms for convex optimization in the context of recent history of the modern interior-point methods. I will focus on some breakthroughs in the area and their theoretical evolution as well as impact.

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### MS66 Optimization and Quantitative Portfolio Management

Optimization models and methods are central elements of quantitative equity portfolio management platforms. They serve as sophisticated tools for transferring the excess return ideas generated through research and testing into portfolios that best represent these ideas. In addition to the standard mean-variance optimization models that are adjusted for trading costs, we will discuss topics such as multi-portfolio optimization (optimizing multiple portfolios simultaneously while minimizing the joint market impact costs) and multi-period portfolio selection.

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### MS66 Two Algorithms for the Minimum Enclosing Ball Problem

Given  $\mathcal{A} := \{a^1, \dots, a^m\} \subset \mathbf{R}^n$  and  $\epsilon > 0$ , we propose and analyze two algorithms for the problem of computing a  $(1 + \epsilon)$ -approximation to the radius of the minimum enclosing ball of  $\mathcal{A}$ . The first algorithm is closely related to the Frank-Wolfe algorithm with a proper initialization applied to the dual formulation of the minimum enclosing ball problem. We establish that this algorithm converges in  $O(1/\epsilon)$  iterations with an overall complexity bound of  $O(mn/\epsilon)$  arithmetic operations. In addition, the algorithm returns a “core set” of size  $O(1/\epsilon)$ , which is independent of both  $m$  and  $n$ . The latter algorithm is obtained by incorporating “away” steps into the former one at each iteration and achieves the same asymptotic complexity bound as the first one. While the asymptotic bound on the size of the core set returned by the second algorithm also remains the same as the first one, the latter algorithm has the potential to compute even smaller core sets in practice since, in contrast with the former one, it allows “dropping” points from the working core set at each iteration. Our computational results indicate that the latter algorithm indeed returns smaller core sets in comparison with the first one. We also discuss how our algorithms can be extended to compute an approximation to the minimum enclosing ball of other input sets. In particular, we establish the existence of a core set of size  $O(1/\epsilon)$  for a much wider class of input sets.

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**MS67****Applications Where GSS Methods are able to Cope with Nonsmoothness**

We consider minimization problems where the objective function is piecewise smooth on a finite family of polyhedra. Problems of this kind arise in many areas of applied sciences, like for example in signal and image restoration, financial mathematics or multivariate data analysis. Some of these problems are in fact piecewise linear and can be solved by linear programming techniques; in other cases however, reformulations as linear programs are impossible because of nonlinear terms in the objective function. Generating set search methods represent a direct and somehow natural approach to cope with this type of nonsmoothness.

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**MS67****Assessing Polymer Extrusion Filter Performance with Gradient-Free Optimization Methods**

Debris filtration is an important component of the polymer fiber melt-spinning process. Filters are replaced once a significant amount of debris accumulates inside the filtration medium; manufacturers also want a minimal amount of debris in the finished product. As each event carries an associated cost, we measure filter performance by combining these objectives. We use a simulation tool to evaluate our functional, thus necessitating the use of derivative-free methods to find parameters that optimize filter performance.

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**MS67****Optimal Design of Municipal Water Supply Portfolios with Implicit Filtering**

In this talk we describe an application of implicit filtering to water resources management. The problem is the optimal design of a portfolio of water rights, leases, and options based on a stochastic model of the water supply. The reliability and conditional value at risk of the design lead to constraints which can only be tested after the simulation is

complete. We can estimate the noise in the function with probabilistic methods and use that information to control the cost of the optimization.

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**MS67****Challenges in Using Derivative-Free Optimization Methods for Scientific Applications**

Optimization has taken an increasingly larger role in many scientific problems today. This is due in large part to the rapid rise of computational modeling and simulation in many scientific fields. As a result, many scientists are now starting to consider using optimization for problems such as the determination of the surface structure of nanosystems, fitting supernova models to data, and the design and operation of particle accelerators. All of the problems share the property that no derivative information is readily available. In this talk, I will discuss some of the challenges and the approaches we have taken for addressing optimization problems arising from these applications.

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**MS68****A Stochastic Multiple-Leader Stackelberg Model: Analysis, Computation, and Application**

We study an oligopoly consisting of multiple leaders and multiple followers that supply a homogeneous product non-cooperatively. Leaders choose their supply levels first, knowing the demand function only in distribution. Followers make their decisions after observing the leader supply levels and the realized demand function. We show the existence and uniqueness of equilibrium, propose a computational approach based on the sample average approximation method, and apply this framework to model competition in the telecommunication industry.

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**MS68****Loss of Efficiency in Quadratic Utility Games**

We study quadratic utility games (for example, Cournot, i.e. quantity competition). We first consider an affine demand-price relation. We present a bound on the loss of efficiency (ie. comparison of system profit between centralized and decentralized settings) that depends on the number of players and the maximum market power of the players. We discuss a setting where sellers have lack of information on the other sellers' constraints. As a result, we provide a bound that is independent of the constraints of the game. Our results apply to competition where multiple products share capacities. We further generalize our results to classes of nonlinear demand functions as well as more general measures of efficiency.

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**MS68****A New Stochastic Game: 2-Stage Perfect Competition with Endogenous Probabilities**

Abstract not available at time of publication.

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**MS68****Empirical Pricing Game with Multiple Equilibria**

We study a Bertrand oligopoly with random coefficients logit demand model. For a given set of parameters, our model would generate multiple price equilibria. We propose an MPEC approach to estimate structural parameters in this model and show that our approach is computationally faster than the widely-used BLP estimator.

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**MS69****Optimization and Inverse Modeling in Metric Spaces**

Reservoir modeling and management calls for the application of non-linear optimization in a highly dimensional and uncertain/stochastic parameter space (the reservoir model space). In this presentation, I formulate the stochastic optimization problem in a metric space defined by a distance between any two model realizations. Using this metric

space, we can reformulate the modeling or optimization problems in a much lower dimension, hence apply standard gradient-based or stochastic optimization techniques effectively.

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**MS69****Inverse Modeling of Oil Reservoirs Using Integrated Data**

The mathematical models used for forecasting oil production involve geological parameters that must be tuned using field data in order to provide meaningful predictions. This calibration process yields large-scale inversion problems that in general have nonunique optimal solutions. In this talk we regularize these problems by jointly considering field data of different kinds, namely cross-well tomographic data and flow measurements. We demonstrate that the use of these two data types provides more realistic geological parameters.

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**MS69****Flooding Optimization of Oil Reservoirs**

We consider model-based techniques to optimize production from oil reservoirs by changing well operating parameters over the full producing life of the reservoir. The models consist of discretized nonlinear diffusion-convection equations. The optimization methods are gradient-based using an adjoint formulation. The large number of control parameters makes the problem-ill posed and we discuss various strategies to regularize the problem.

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**MS69****Efficient Ensemble-Based Closed-Loop Production Optimization**

In this paper, we describe a new method for closed-loop optimization, which combines ensemble-based optimization with the Ensemble Kalman Filter (EnKF) for data assimilation. The EnKF adjusts the reservoir models to honor observations and propagates the uncertainty in time. An ensemble-based steepest ascent method is used to optimize the expectation of the net present value based on the updated reservoir models. The method is illustrated with a waterflood example.

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**MS70****Ab Initio Molecular Dynamics and Electronic Structure Simulations That Involve Thousands of Atoms: Algorithmic, Numerical and High Performance Computing Challenges**

Electronic structure calculations from first principles have revealed a remarkable wealth of information concerning important properties of materials and nano-structures. Taking advantage of the advances in computing (software and hardware) and the advent of massive parallelism the future looks even more promising. We will show that moving to next generation simulations with tens of thousands of atoms requires the efficient combination of powerful optimization and numerical algorithms with the latest paradigms of parallel computing.

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**MS70****Iterative Algorithm for Wave Functions Optimization in Density Functional Theory: Inexact Newton with Anderson Acceleration**

We put a mathematical framework around a numerical algorithm we have used to solve electronic structure problems in recent years. The approach is described as a subspace accelerated inexact Newton inspired by Fokkema et al. It makes use of the acceleration scheme introduced by Anderson. It is applicable in  $O(N)$  algorithms where electronic orbitals are confined to localization regions.

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**MS70****Experience with Gradient-Based Optimization Methods for Energy Minimization in Electronic****Structure Calculations**

The problem of finding mechanically stable configurations of materials is a common task in computational materials science, physics, chemistry, and biology. This corresponds to finding the nearest material configuration, with minimum potential energy, from a given configuration. There are many well-established gradient-based optimization methods (including quasi-Newton, conjugate gradient, and others) available for this task. In this talk, we consider such methods and compare results obtained from using these methods to find mechanically stable material configurations.

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**MS70****Numerical Algorithms for Total Energy Minimization in Electronic Structure Calculation**

One of the fundamental problems in electronic structure calculations is to determine the electron density associated with the minimum total energy of a molecular or bulk system. The total energy minimization problem is often formulated as a nonlinear eigenvalue problem and solved by an iterative procedure called the self-consistent field (SCF) iteration. In this talk, I will describe SCF and explain why it can fail to converge. I will discuss techniques for improving the convergence of SCF and present an alternative algorithm that minimizes the total energy directly.

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**MS71****OB1: The Computational History**

In 1988, Lustig, Marsten and Shanno began a collaboration to develop OB1, which was used to develop numerous insights into the computational aspects of primal-dual interior point methods for linear programming. In this talk, we will review the history of these developments and its impact on computational linear programming.

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**MS71****Lagrangian Transformation in Constrained Optimization**

A class of strongly concave and smooth enough functions  $\psi : \mathcal{R} \rightarrow \mathcal{R}$  is used for transforming terms of the Classical

Lagrangian related to constraints. The resulting function is used for developing two classes of multipliers methods. The first class is equivalent to the Interior Prox methods with Bregman distance function for the dual problem while the second is equivalent to the Interior Quadratic Prox in the rescaled dual space. We use the equivalence for proving convergence and estimating the rate of convergence of the multipliers methods.

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### MS71

#### Using MPECs to Derive Implied Binomial Trees

It is widely recognized that the assumption of constant volatility in the Black-Scholes options pricing model is incorrect. One way to modify Black-Scholes is to use a model with local volatility. However, in the case of American options, deriving the implied parameters for a binomial tree when volatility is no longer assumed to be a constant proves to be a difficult proposition, with much attention given in the literature. Here we consider an approach to deriving implied binomial trees by solving a mathematical program with equilibrium constraints, or MPEC.

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### MS72

#### A PDE-Constrained Approach to Electrostatic Optimization of Biomolecules

A convex quadratic program has been derived for optimizing the electrostatic component of binding free energies between molecules, and experimental validation of the formalism has demonstrated its usefulness in molecular analysis and design. We have developed a novel PDE-constrained formulation that dramatically reduces the computational cost for these problems, outperforming the original method and also standard PDE-constrained techniques. Biological examples demonstrate the method's viability and performance, as well as issues faced generally by PDE-constrained approaches.

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### MS72

#### Optimization Methods in Applied Protein Design

The definition of an appropriate inverse problem to the protein structure prediction problem, coupled with the application of remarkably effective tree pruning and search algorithms, has made computational protein design a reality. Here, we will discuss the optimization techniques underlying applied protein design, as well as an application involving the simultaneous design of optimal genetic

(DNA) and amino-acid sequences for expressed natural or artificial proteins.

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### MS72

#### Monte Carlo-Based Prediction of Ligand Binding Geometries

A wealth of computational strategies is available for predicting the binding site and affinities of a putative ligand inside a target receptor. Although numerous techniques have been reported for the orientation of ligands or fragments thereof, few methods have delved into improving the accuracy of generating reliable ligand conformations within predicted binding modes. In an effort to comprehensively sample the torsion space available to a flexible ligand and focus on low energy conformations, a recursive, Metropolis Monte Carlo-based rotamer design protocol has been developed. This approach recursively samples adjacent rotatable bonds from a defined anchor and directs the search along low energy pathways, such that high-affinity conformations of the ligand can be identified. Furthermore, this program applies spatial constraints within the search that restrict the solutions to structurally dissimilar conformations, thus encouraging diversity in the solution set. The performance of moleculeGL has been evaluated for a set of 55 cocrystals, with the number of rotatable bonds for the ligands varying from 2 to 32. About 85% of the structures predicted, starting from an arbitrary ligand conformation, are within 2.0 Å<sup>2</sup> root mean square displacement with respect to the crystal structure. This high level of accuracy starting from arbitrary ligand conformation suggests the program's applicability to the design of pharmacophore substituents, for which the position of a chemically-active pharmacophore is well-known.

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### MS72

#### Electrostatic Optimization in Drug and Drug Cocktail Design

In this talk, I will outline two major optimization techniques as they apply to drug design. The first technique determines the electrostatic properties of a hypothetical drug molecule that binds as tightly as possible to its target, using a continuum electrostatics framework. This method has been used to improve and analyze existing molecules, and it can potentially be used in design. The second technique uses integer-programming based methods to select or design drug cocktails that can collectively target a rapidly-mutating agent. Such methods could be useful in a system with multiple target variants, such as HIV or certain forms of cancer. Finally, these two techniques can be combined to further understand the physical determinants of molecules and drug cocktails capable of recognizing rapidly mutating

drug targets.

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### MS73

#### Shape Optimization for Biocompatibility in Implantable Blood Pump Design

Several challenges and methods in biomedical flow device design are described. The objective often involves the unique behavior of blood as the flowing medium, necessitating, e.g., accurate modeling of cell damage. The complex constitutive behavior, in particular shear-thinning, may affect the outcome of shape optimization more than it affects direct flow analysis. Finally, target applications often involve intricate time-varying geometry, and thus, realistic solutions can be only obtained on high-performance parallel computers.

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### MS73

#### PDE Constrained Optimization with Uncertain Input: Optimal Probe Location for the Radio-Frequency Ablation

The radio-frequency (RF) ablation is a promising minimally invasive treatment for lesions in the human liver: A probe containing electrodes is placed in the tumor and connected to a generator. Consequently an electric current flows through the tissue and heats it up to temperatures of more than 60 degrees Celsius. This leads to a coagulation of the cell's proteins and thus a destruction of the malignant tissue. The success of the treatment heavily depends on a variety of patient-individual quantities, e.g. the local structure of the vascular system and material parameters like the water content of the tissue, its heat-capacity, its heat- and electric-conductivity, etc. So in the interest of the patient a thorough planning of the therapy must be made, yielding an optimal position and orientation of the probe, and taking these important patient-individual properties into account. The talk focusses on models for the optimization of the RF-ablation. To take the uncertainty associated with patient individual material parameters into account, we formulate the forward problem in terms of a stochastic PDE. Consequently we consider objective functions which involve stochastic modes of the resulting probability distribution of the heat distribution. We present the

corresponding optimality systems and an algorithm that uses stochastic collocation to evaluate stochastic integrals.

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### MS73

#### Shape Optimization Under Uncertainty – A Stochastic Programming Perspective

We present an algorithm for shape-optimization under stochastic loading, and representative numerical results. Our strategy builds upon a combination of techniques from two-stage stochastic programming and level-set-based shape optimization. In particular, usage of linear elasticity and quadratic objective functions permits to obtain a computational cost which scales linearly in the number of linearly independent applied forces, which often is much smaller than the number of different realizations of the stochastic forces. Numerical computations are performed using a level-set method with composite finite elements both in two and in three spatial dimensions.

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### MS73

#### Gradient Smoothing and Hessian Approximation for Aerodynamic Shape Optimization in Oneshot

Numerical optimization in general and aerodynamic shape optimization in specific is a field which has seen much progress in the past decade. Since the adjoint approach makes the computation of the gradient in principle independent of the number of design parameters, it is appealing to use a high resolution in the optimization process. Here we parameterize the shape itself by the boundary mesh nodes for the aerodynamic flow problem. This, however, may introduce high frequency noise in the shape, which can be circumvented by appropriate means. The Hessian for these problems is usually a pseudo-differential operator and knowledge of this operator can be used not only to cure the loss of regularity but also to accelerate the convergence of a gradient based optimization approach. We propose using the analytical shape derivative on the surface nodes of the mesh, combined with the adjoint approach in the flow field, which completely decouples the optimization from the mesh generation. The implementational details and the efficiency of the resulting numerical methods for aerodynamic shape optimization are demonstrated in numerical examples of optimal wingcross-sections for Navier-Stokes flow.

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MS74

### Solving Mixed-Integer Nonlinear Problems of Black-Box Type in Engineering Applications with Surrogate Functions

Simulation based optimization becomes increasingly important in engineering applications, especially the need to handle real-valued as well as integer-valued variables is emerging. In this talk we give an introduction on this kind of optimization problems and present an optimization approach based on sequentially updated surrogate functions. Numerical results obtained with the proposed approach will be discussed for numerical examples from engineering applications where computational expensive, nonsmooth, black-box type mixed-integer nonlinear optimization problems arise.

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MS74

### A Framework For Particle Swarm Optimization for Mixed-Integer Problems Using Surrogate Models

Particle Swarm Optimization is a type of population based, heuristic optimization technique shown to perform well for noisy, nonconvex objective functions containing many local minima. To improve the computational efficiency of the PSO algorithm, we propose a hybrid method that incorporates a surrogate oracle to help update the swarm position. Furthermore, since problems requiring population based methods are often expressed as mixed integer problems, we also incorporate a modified PSO algorithm to directly handle integer variables.

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MS74

### The Influence of Different Experimental Designs on the Performance of "Surrogate Model"-Based Solvers

When dealing with costly (expensive to evaluate) objective functions, one alternative is to use a surrogate model (response surface) approach. A common feature for all such methods is the need of an initial set of points, or "experimental design", in order for the algorithm to get started. The question is how to choose a good experimental design, since the behavior of the algorithms often depend heavily

on this set of initial points

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MS75

### Interior Decomposition Methods for Two-Stage Stochastic Programming

We present theoretical and computational results on decomposition methods for solving two-stage stochastic programming problems. In particular, we show that these methods have the same first-stage worst case iteration complexity as their extensive formulation. Moreover, by introducing a novel concept of self-concordant random variables, we show that under a probabilistic assumption the number of iterations in a weighted decomposition method is independent of the number of scenarios. Additional theoretical and computational results will be presented depending on the progress.

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MS75

### Active Set Algorithms for Conic Programming

It is known that an upper bound can be placed on the rank of an optimal solution to a semidefinite program. An active set method can then be designed which works with semidefinite programs of size no larger than a small multiple of this bound. We discuss approaches where a high dimensional cone is approximated by a lower dimensional cone, with the lower dimensional cone updated from iteration to iteration.

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MS75

### On Solving Specially Structured Large SDPs Using IPMs

The stability conditions for spatially-distributed control systems give rise to large semidefinite programs with specific block angular structure. The standard first-order Dantzig-Wolfe decomposition techniques are usually employed. We explore related smooth counterparts that can be solved using interior-point techniques whose subproblems are solved approximately and still promise faster asymptotic convergence, as well as improved global con-

vergence.

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### MS75

#### A Parallel Interior Point Decomposition Algorithm for Sparse Polynomial Optimization

Recently, Waki et al. have proposed a hierarchy of structured semidefinite programming (SDP) relaxations in the "block-angular" form for sparse polynomial optimization problems. We discuss an interior point decomposition algorithm for solving these block-angular SDPs in a parallel and distributed high performance computing environment. We will also present our computational experiences with the algorithm on the distributed "Henry2" cluster at NC State University.

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### MS76

#### Improving the Homogeneous Self-Dual Interior-Point Method Via Projective Transformation

The homogeneous self-dual (HSD) embedding model is both a theoretically interesting methodological tool as well as a practical way to solve conic convex optimization problems via interior-point methods (IPMs). Herein we study stopping rules for IPMs for the HSD model, and their implications and connections to the complexity theory of conic convex optimization. We also develop a projective transformation methodology for improving the theoretical performance of IPMs for solving HSD models. Computational results validate the practicality of our approach.

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### MS76

#### Bregman Iterative Algorithms for Compressed Sensing and Matrix Rank Minimization

We propose efficient methods for solving the Basis Pursuit problem  $\min\{\|u\|_1 : Au = f, u \in \mathbf{R}\}$ , based on Bregman iterative regularization, that obtain an accurate solution after solving only a very small number of instances of the unconstrained problem  $\min_u \mu\|u\|_1 + \frac{1}{2}\|Au - f^k\|_2^2$ . We prove that an exact solution is obtained in a finite number of steps, and present numerical results on huge compressed sensing applications where matrix-vector operations involving  $A$  and  $A^T$  can be computed by fast

transforms. We also, describe extensions to matrix rank minimization.

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### MS76

#### Elimination of Free Variables for Solving Semidefinite Programs Efficiently

An important issue in interior point methods for semidefinite programs (SDPs) is handling of free variables. Recently, Kobayashi, Nakata, and Kojima proposed a method that transforms a given SDP with free variables into a standard equality form SDP by eliminating free variables. A disadvantage of the method is that the sparsity of the data matrices of the SDP may be destroyed. We discuss how the sparsity in the transformation can be maintained and show some numerical results.

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### MS76

#### Competitive Market Equilibrium Computing

We present a fully polynomial-time approximation scheme for computing a symmetric Leontief economy equilibrium, that is, an exchange market equilibrium model with symmetric Leontief's utilities; where the equilibrium set can be non-convex and non-connected. We report our preliminary computational results using an interior-point potential reduction algorithm for non-convex quadratic programming.

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**MS77****Parallel Derivative-free Non-Monotonous Algorithms for Bound Constraint Optimization**

A new parallel algorithm is proposed that solves an optimization problem subject to bounds on the variables. The algorithm assumes no accurate derivative information, it is non monotonous and converges under suitable assumptions to a point satisfying the first order necessary condition for optimality. Nonetheless, it includes ingredients to scape from local optima. The algorithm has three distinctive properties: a) A processor broadcasts only those points on which the processor is unable to make any improvement (partially blocked points), b) Directions of search are not assigned to processors. They look for improvement on a given subspace, and c) Convergence is not impaired due to processors breakdowns. If only one processor is alive, it essentially executes a sequential algorithm. Preliminary numerical experiments on classical test problems are encouraging. We noticed that the number of function evaluations may decrease when augmenting the number of processors.

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**MS77****Adaptive Radial Basis Algorithms (ARBF) for Expensive Global MINLP Optimization**

Improvements of the adaptive radial basis function algorithm (ARBF) for computationally costly optimization are presented. A new target value search algorithm and modifications to improve robustness and speed are discussed. The algorithm is implemented in solver ARBFMIP in the TOMLAB Optimization Environment (<http://tomopt.com/>). Solvers in TOMLAB are used to solve global and local subproblems. Results and comparisons with other solvers are presented for global optimization test problems. Performance on costly real-life applications are reported.

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**MS77****Extensions of Orbit to Computationally Expensive****Global Optimization**

ORBIT (Optimization by Radial Basis Function Interpolation in Trust Regions) is an RBF model-based algorithm for unconstrained local derivative-free optimization of computationally expensive functions. In this talk we explore preliminary extensions of ORBIT to the global optimization setting. The RBF models employed allow us to take advantage of previously-evaluated points, a particularly valuable property when the function of interest is computationally expensive. We will report on initial testing of some of these extensions. -

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**MS77****Extension of Pswarm to Linearly Constrained Derivative-Free Global Optimization**

PSwarm was developed originally for box-constrained global optimization of functions without derivatives. PSwarm polls as in coordinate search and incorporates in the search step a particle swarm scheme for dissemination and global optimization. PSwarm has just been extended to handle general linear constraints. The poll step incorporates now linear generators for the tangent cones including a provision for the degenerate case. The search step has also been adapted accordingly. In particular, the initial population for particle swarm is computed by first inscribing an ellipsoid of maximum volume to the feasible set. We have again compared PSwarm to other global solvers and the results confirm its competitiveness in terms of efficiency and robustness. If time permits we will discuss the current application of PSwarm to identify optimal parameters in star evolution models in astrophysics.

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**MS78****Extended Mathematical Programs**

Abstract not available at time of publication.

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**MS78****Generalized Disjunctive Programming and EMP**

Abstract not available at time of publication.

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**MS78****Dynamic Games and EMP**

Abstract not available at time of publication.

Kenneth JuddHoover Institution  
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Abstract not available at time of publication.

Alexander MeerausGAMS Corporation  
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Oil and gas pipelines carry the bulk of the world's energy, and are a rich source of challenging optimization problems. Three common properties are: (A) Objectives and constraints are derived from simulation software, (B) The simulation software itself may itself involve numerical solution of optimization problems, and (C) The results of the optimization are often needed directly, but in some decision-making contexts they are of greatest value when used quite indirectly. We present examples to illustrate the above properties, and discuss a few useful algorithms and methodologies to address some of the issues that arise in multi-level optimization/simulation of this sort.

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Sanjay Yadav

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The Troll Oil field, located in the North Sea, is one of the worlds largest subsea developments. Present Troll production is governed by over 100 subsea wells, producing into 27 clusters and with more than 200 kilometers flexible flow lines at water depths of 320 to 350 meters. Troll production is limited by the process gas-handling capacities and by flow line capacities. The main optimization variables in the system are thus the choke valve positions, the gas lift rates, and the well routing. In mathematical terms, the problem to be solved is a large-scale mixed-integer non-linear problem (MINLP). A system of in-house and commercial tools is used to model and solve this challenging problem with satisfactory results. The system is currently

in use by the production engineers at the Troll field.

Marta Duenas-DiezStatoil-Hydro  
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An important optimization problem in oil field operations is the determination of optimal well settings (pressures, flow rates) to maximize oil production. In recent work we applied gradient-based methods, with gradients obtained from adjoint solutions, for these problems. These algorithms are efficient but require access to source code for the forward model and detailed code development. In this talk, we consider other algorithms for production optimization and compare their performance with the adjoint procedure.

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David Ciaurri, Obi Isebor

Stanford University  
david.echeverria@stanford.edu, oisebor@stanford.edu**MS79****Adjoint Calculations for a Reservoir Management Problem**

We first present an optimization approach based on an algebraic surrogate model for the reservoir and outline its strength and deficiencies. Then we will present a model derived from a PDE-based reservoir simulation. Finally, we demonstrate how to calculate adjoints and gradients for a time dependent optimal control problem using different time discretization schemes and present numerical results.

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Matthias Heinkenschloss

Rice University  
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Gossip algorithms have recently received significant attention, mainly because they constitute simple and robust algorithms for distributed information processing over networks. However, for many topologies that are realistic for wireless ad-hoc and sensor networks, the standard nearest-neighbor gossip is diffusive in nature and converges very slowly. A series of recent results have successively improved the convergence time of such algorithms. This talk



will review this recent work, connections to eigenvalues of large random matrices, and further extensions to general message passing algorithms for statistical inference in distributed environments.

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### MS80

#### Computing Sparse Generators of Homology Groups in Simplicial Complexes

Computation of topological invariants of networks represented by simplicial complexes have become a useful tool in diverse applications such as verification of dynamic coverage in sensor networks and target enumeration. Simplicial complexes are the main object of study in algebraic topology and can be thought of as generalizations of graphs for modeling higher order relations, as opposed to just binary ones. One central step in applying such tools is computing generators of homology groups which represent various kinds of "holes" in a network. In this talk, we present an optimization based approach to distributed computation of the sparsest generator for the homology groups of simplicial complexes. First we show how this problem is related to the problem of localizing coverage holes as well as the problem of finding a minimal cover in a sensor network. Next, we show that the problem can be formulated as an integer programming problem which can be relaxed to a linear program. We then show that the relaxation is exact, and therefore, one can efficiently compute the minimal generator of the homology groups. We also present a subgradient method for finding the minimal generator in a distributed fashion.

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### MS80

#### Distributed Multi-Agent Optimization

We present a distributed computational model for optimizing a sum of convex objective functions corresponding to multiple agents. In this model, each agent minimizes its own local objective while exchanging the estimate information with the neighbors according to some rules. For

solving this (not necessarily smooth) minimization problem, we consider a sub-gradient method that is distributed among the agents. We study convergence properties and provide convergence rate estimates for the method. Our convergence rate results explicitly characterize the tradeoff between a desired accuracy of the generated approximate optimal solutions and the number of iterations needed to achieve the accuracy. We also study the effects of quantization, and provide convergence results and rate estimates for a quantized method.

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### MS80

#### Matrix Splitting Methods for Distributed Optimization Problems

We consider the solution of distributed optimization problems through the use of splitting approaches. Specifically, we provide conditions under which the subproblems in such schemes can be solved using matrix splitting methods. Furthermore limited synchronization through linesearch or trust region methods will be discussed. Some preliminary numerical results are provided.

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### PP0

#### Optimization Method Applied to Analysis of Surface Water Quality in Eastern Massachusetts

The USGS National Water-Quality Assessment (NAWQA) Program provides long-term measurements on streams, rivers, ground water, and aquatic systems. Using time series data from Eastern Massachusetts streams, we analyze the current state of surface water, changes in time and dependence on land use, precipitation regime, and possible

other natural and human influences. We use optimization techniques to address the robustness of the statistical characterization of relationships among various measured dissolved components and other physical parameters.

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#### PP0

##### **Variational Formulation of Dynamic Oligopolistic Market Equilibrium Problem and Computational Procedure**

The aim of the talk is to present a variational inequality formulation of the dynamic oligopolistic market equilibrium problem. Moreover existence theorems of a dynamic solution to the associated evolutionary variational inequality is showed under general assumptions and a continuity theorem of the solution is established. Then, we apply the regularity result to compute the solution of the dynamic oligopolistic market equilibrium problem by means a discretization procedure.

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#### PP0

##### **Competition and Efficiency in Communication Networks**

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#### PP0

##### **The Neos-Wiki – An Open-Access Online Optimization Resource.**

The new NEOS-wiki places the "NEOS Guide to Optimization". The aim of the NEOS-wiki is to become a focal point for optimization resources by extending the extensive range of resources in the old guide, such as the case studies, the optimization FAQs, and the software guide. This poster launches our campaign to encourage new contributions from the optimization community. See <http://wiki.mcs.anl.gov/NEOS/>

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#### PP0

##### **A Primal-Dual Method for Nonlinear Equality Constraints Programming**

We analyze the behaviour of the Newton method applied to a sequence of perturbed optimality systems that follow from the quadratic penalty approach. We show that the usual requirement of solving the penalty problem at an arbitrary given precision may be replaced by a less stringent criterion, while guaranteeing the global convergence. Local and global convergence results are presented, as well as some preliminary experiments.

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**PP0****An Improved Approximation Algorithm for the Column Subset Selection Problem**

Given  $A \in R^{m \times n}$  and  $k \ll n$ , the Column Subset Selection Problem is: pick  $k$  columns from  $A$  to form  $C \in R^{m \times k}$ , such that to minimize  $\|A - CC^+A\|_\xi$ , for  $\xi = 2$  or  $F$ . This combinatorial optimization problem has been exhaustively studied within the numerical linear algebra and the theoretical computer science communities. Current state-of-the-art approximation algorithms guarantee

$$\|A - CC^+A\|_2 \leq O(k^{\frac{1}{2}}(n-k)^{\frac{1}{2}})\|A - A_k\|_2,$$

$$\|A - CC^+A\|_F \leq \sqrt{(k+1)!}\|A - A_k\|_F.$$

Here, we present a new approximation algorithm which guarantees

$$\|A - CC^+A\|_2 \leq O(k^{\frac{3}{4}} \log^{\frac{1}{2}}(k)(n-k)^{\frac{1}{4}})\|A - A_k\|_2,$$

$$\|A - CC^+A\|_F \leq O(k\sqrt{\log k})\|A - A_k\|_F,$$

and *asymptotically* improves upon the previous results.  $A_k$  is the best rank- $k$  approximation to  $A$ , computed with the SVD

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**PP0****Greedy is Good, But Branching is Better: A Local-Ratio Style Improvement for Hitting Set of Bundles Problem**

In this work, we extend the approximation analysis of the Hitting Set of Bundles (HSB) problem using a greedy, rather than LP-based approach. This combinatorial framework yields a theorem, regarding the structure of the worst-case instances of HSB, that leads to a simple branching improvement scheme. We prove that this branching approach yields the best-known approximation ratio on an important class of HSB problems, and present experimental results for more general instances.

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**PP0****A p-Cone Sequential Relaxation Procedure for 0-1 Integer Programs**

Given a 0-1 integer programming problem, several authors have introduced sequential relaxation techniques – based on linear and/or semidefinite programming – that generate the convex hull of integer points in  $n$  steps. In this paper, we introduce a sequential relaxation technique based on  $p$ -order cone programming. We prove that our technique generates the convex hull asymptotically and generalizes several existing methods. We also show that for  $p=2$  our method enjoys a better theoretical iteration complexity.

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**PP0****Face Recognition Using Order-Value Optimization**

Order-value optimization (OVO) is a generalization of the minimax problem; it consists in the minimization of the functional value that ranks in the  $p$ -th place. In this work, an application of OVO optimization to the problem of finding hidden patterns in data sets is described. In this application, one wants to identify a probe face image (rotation, scaling, and displacement) of a gallery (face set of known faces). Numerical experiments are presented.

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**PP0****Variational Shape Optimization with Applications in Image Processing**

We describe a novel variational shape optimization method, which closely follows the continuous structure of the geometric optimization problem. We express the geometry explicitly and discretize the formulation with finite elements. In this way we also easily incorporate space adaptivity to tune accuracy and computational cost. A distinct feature of our method is the possibility to obtain specially designed descent directions by varying the associated scalar products at the continuous level. We demonstrate our method in two image processing problems: the geodesic active contour model for boundary detection and the Mumford-Shah model for simultaneous image segmentation and smoothing.

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### PP0

#### Newton's Method, Chebychev, Halley, and Beyond to Minimize $f(x)$ .

We present the classical Newton, Chebychev and (super) Halley iterative methods in the context of nonlinear unconstrained optimization. We observe that Newton's and Chebychev's methods may be obtained from an extrapolation interpretation. On the other hand, both the Chebychev and Halley classical methods use similar expressions involving third order derivative of the objective  $f$ . We present fourth order methods inspired by those third order variants. For this poster presentation, we insist on the intuition underlying our developments.

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### PP0

#### Multiple Return Estimation for Robust Portfolio Optimization

Classical mean-variance formulations for portfolio optimization problems depend on accurate and consistent estimates for expected returns and risks of securities included in the portfolio selection model. A comparison of various estimation techniques, however, shows that the predicted performances typically vary widely and, thus, prompts to rethink the concept of a robust portfolio. Using a multi-scenario multi-objective modeling approach that incorporates several return estimates, new formulations for robust portfolio optimization are proposed and illustrated on examples.

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### PP0

#### Packing Cylinders on a Cylinder with Contact Constraints

The problem of cylinder packing is investigated. The specific problem is to find the optimal packing of congruent cylinders about a core cylinder of arbitrary dimensions. The constraint is that their circular face must keep in contact with the core cylinder. Mathematically, a lower and upper bound is determined. A quantitative result is also found using a modified genetic algorithm which reproduces published results for the problem of packing congruent circles within a circle.

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### PP0

#### Approximation of Impulsive Solutions in Fully Convex Optimal Control Problems

Optimal control and calculus of variations problems with joint convexity are considered, where the associated Hamiltonian is possibly extended-real valued. As a consequence, optimal trajectories become arcs of bounded variation. Using Goebel's smoothing technique for the Hamiltonian, conditions under which solutions of the smoothed problem converge to solutions of the original problem are identified.

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### PP0

#### FDMA Based Optimality Analyses and Algorithms

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### PP0

#### Global Versus Local: An Analysis of the Selfish Behaviors in Spectrum Management

In this talk we shall discuss how each individual's optimum behavior can alter the spectrum allocation in a multi-user communication system. We show that if the users respond optimally to the \*history\* of the behavior of all other users, then the overall performance of the system can be improved. This suggests that it pays to educate the users and manage the public information, notwithstanding the selfish nature of the individual users. In other words, one kind of "educated selfishness" may be better than the uninformed one, in the interest of global optimization.

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### PP0

#### A One-Unit System Supported by a Spare and Serviced by Two Repair Persons

A one-unit system is supported by an identical spare unit, and is serviced at a facility where there is an in-house regular repair person who performs a perfect repair.

Should the repair take longer than a predetermined patience time, or should the other unit also fail, immediately an expert repair person is called in to take over the repairing task. We call a model MER(multiple expert repair)/SER (single expert repair if the expert, once called in, will fix all/only one failed unit before leaving. We use RPT(random patience time)/DPT(deterministic patience time) to denote the case when the patience time is chosen to be random/deterministic. Sridharan and Mohanavadivu (1998) proposed and study the SER-RPT model. We study 4 models: MER-RPT, SRE-RPT, MER-DPT and SER-DPT and derive the optimal conditions for limiting availability and profit per unit time for choices between these 4 models.

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#### PP0

##### Optimization Approaches For The Inverse Elasticity Problem

This poster will focus on the inverse problem of identifying Lamé parameters in elasticity. This problem has found interesting applications in elasticity imaging (in locating cancerous tissues, and other abnormalities). We present several optimization based approaches that can be used to solve the inverse elasticity problem. Adaptive finite element methods are used in computations.

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#### PP0

##### Identification of Transport Parameters of Soils From Column Tests

Application of optimization techniques for identification of transport parameters of soils: effective porosity, dispersivity and sorption factors is discussed. The source of data are results obtained from column tests for inert and sorbing ions migrating through different soils. The solutions of pde problems are based on finite element method for non-steady transport. Different loading modes and models of boundary conditions as well as scale effect are considered.

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#### PP0

##### Robust Optimization for Biological Network Calibration

Calibrating chemical-kinetics based differential equation models for biological networks is a task that is often made difficult by the limited amount of available experimental data. When an additional robustness constraint is included in the optimization problem, results suggest that the calibration can be made far less sensitive to a-priori parameter estimates. Research thus far has been conducted primarily in the context of signal transduction pathways, such as the mitogen-activated protein kinase pathway.

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#### PP0

##### Pennon 1.0 - A Code for Nonlinear Semidefinite Programming

We will present PENNON 1.0 - the first release of the code for solving mathematical optimization problems with real and matrix variables, smooth nonlinear (nonconvex) objective and smooth nonlinear equality and inequality constraints. All functions may depend on both types of variables. Additionally, the matrix variables may be subject to spectral constraints, in particular, to positive semidefinite constraints. Matlab and extended AMPL interface allow the user to formulate the problems easily. We will present a few of numerous applications of the code.

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#### PP0

##### Optimization of Cosmological Surveys

Due to the huge investment in next-generation Cosmological surveys aimed at answering fundamental questions about the Universe, successful optimization of their design is vital. We consider an example, the optimization of the

\$50M WFMOS survey, highlighting the impact of uniquely developed algorithms for this purpose which involves multiple design variables.

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## PP0

### **FASTr: A Filter Active - Set Trust - Region Framework**

We describe a new open-source library for solving large-scale nonlinear optimization problems. The library implements a flexible trust-region framework. Global convergence is promoted with a filter or a recently proposed tolerance tube. The framework includes SQP, SLP-EQP, and regularized LP methods, and allows a range of QP/LP subproblem solvers. Numerical experience on the CUTER test set is presented.

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## PP0

### **An Integrated Electric Power Supply Chain and Fuel Market Network Framework: Theoretical Modeling with Empirical Analysis for New England**

We develop a novel variational inequality-based electric power supply chain network model with fuel supply markets that captures both the economic transactions in energy supply chains and the physical transmission constraints in the electric power network. We then apply the model to a specific large-scale case, the New England electric power supply chain, consisting of 6 states, 5 fuel types, 82 power generators, with a total of 583 power plant and generator combinations, and 10 demand market regions. We show that the model very closely predicts the actual prices.

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## PP0

### **Comparison of Optimization Methods on the Inverse Dynamics Musculoskeletal Problem in Biomechanics**

A comparison study of a SQP and Gauss-Newton method is

presented for solving the inverse dynamics musculoskeletal problem, formulated as an optimal control problem with direct transcription. This kind of problem roughly consists of computing muscle and reaction forces from motion data. Here the problem is formulated with objective function as the least square difference between computed motion and measured motion and the equations of motion and muscle dynamics equation as constraints.

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## PP0

### **An Interior Point Method for the Hydro Power Generation Scheduling with Nonlinear Network Constraints**

Scheduling generation in hydro-thermal power systems is a large-scale, stochastic, nonlinear, and nondifferentiable problem. Traditional modeling proposed so far inserts non-convexity, adding unnecessary complexity to the problem. This work presents a new convex model that adds nonlinearity to network constraints related to the electrical balance equations. To solve the problem, an interior point method that exploits particularities inherent to this class of problems is presented, drastically reducing the number of matrix operations.

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## PP0

### **Intelligent Robust Optimisation for Power Capacity Expansion**

The aim of this study is to identify an optimised capacity expansion plan for a power system based on future uncertain variables such as demand. To achieve this objective, this research uses the concept of scenario planning to consider different scenarios for the future. The proposed framework develops a scenario generator by using artificial neural networks and fuzzy logic. Then, an optimisation method called intelligent robust optimisation finds a robust investment option based on the different future scenarios.

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### PP0

#### Subdifferentials Associated with Some Quasiconvex Dualities

We study some subdifferentials for generalized convex functions, using some dualities and conjugacies. We establish some links between concepts of generalized convexity and these subdifferentials. We devise some optimality conditions for constrained optimization problems and the dual problems. Key words: conjugate, duality, generalized differential, optimality conditions, subdifferential. Mathematics Subject Classification: 26B25, 49K26, 90C26

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### PP0

#### An Efficiency Measure for Dynamic Networks with Application to the Internet and Vulnerability Analysis

We propose an efficiency measure for dynamic networks, including the Internet, based on evolutionary variational inequalities, which captures demands, flows, and costs/latencies over time, and which allows for the identification of the importance of the nodes and links and their rankings. We provide both continuous time and discrete time versions of the efficiency measure. We illustrate the efficiency measure for the time-dependent (demand-varying) Braess paradox and demonstrate how it can be used to assess the most vulnerable nodes and links in terms of the greatest impact of their removal on the efficiency/performance of the dynamic network over time.

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### PP0

#### LSTRS: MATLAB Software for Large-Scale Trust-Region Subproblems and Regularization

We describe a MATLAB implementation of the LSTRS method proposed in M. Rojas, S.A. Santos and D.C. Sorensen. A new matrix-free algorithm for the large-scale trust-region subproblem, SIAM J. Optim., 11(3): 611-646, 2000. LSTRS is an iterative method that requires the solu-

tion of an eigenvalue problem at each step. The method is limited-memory and matrix-free. We describe the method, the software and present examples of its use as well as numerical results on large regularization problems.

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### PP0

#### A Solution for Large-Scale Nonlinear Least-Squares with Simple Bounds

We present an algorithm for bound-constrained nonlinear least-squares that solves a sequence of bound-constrained linear least-squares subproblems. The subproblems are handled efficiently by the subproblem solver. Compared with other constrained nonlinear optimization methods, this approach avoids forming the normal equations and only requires matrix-vector products. Numerical experiments are presented to illustrate the effectiveness of this approach.

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### PP0

#### Model-Based Optimal Control of Self-Organized Biochemical Systems

We demonstrate how model-based optimal control can be exploited in biological and biochemical modeling applications focusing on the analysis and the target oriented manipulation of self-organized dynamical systems. We show that the formulation of inverse problems can provide important insight into dynamic regulations of self-organized cellular signal transduction. We apply mixed-integer optimization and Bock's direct multiple shooting method to a circadian oscillator model. The resulting chronomodulated pulse-stimuli schemes lead to restoration of the circadian rhythms.

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## PP0

### Geometric Optimization on the Manifold of Rank Constrained SPD Matrices

We present geometric optimization algorithms that approximate solutions of matrix equations by low-rank SPD matrices. By exploiting the fact that the set of rank constrained SPD matrices is a smooth manifold, we can lift the cost function to the tangent space of the manifold. This allows us to circumvent the curse of dimensionality involved in these matrix equations. The geometry and implementation of the manifold as well as trust-region methods are discussed.

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## PP0

### Environmental and Cost Synergy in Supply Chain Network Integration in Mergers and Acquisitions

In this paper, we quantify and assess, from a supply chain network perspective, the environmental effects resulting when a merger or acquisition occurs and the resulting synergy from possible strategic gains. We develop a multicriteria decision-making supply chain network framework that captures the capacitated economic activities of manufacturing, storage, and distribution pre and post the merger. The variational inequality-based models yield the system optima associated with the minimization of the total costs and the total emissions under firm-specific weights. We propose a synergy measure that captures the total generalized cost. We then apply the new mathematical framework to quantify the synergy obtained for specific numerical examples.

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## PP0

### A Continuous Approach for Max K-Cut and Related Zero-One Quadratic Programs

We give improved deterministic approximation scheme for max K-cut for small values of K. We also present a simple algorithm for max K-cut which converges to a local optimal solution. These approaches are extended to certain classes of zero-one quadratic programs, including the independent set problem.

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## PP0

### Analysis of Competitive Economy Equilibrium Solution for Spectrum Management

This study analyzes the competitive economy equilibrium solution for spectrum management in a weak-interference market. Experimental results indicate that the competitive economy equilibrium solution can provide an efficient spectrum allocation to achieve a higher social utility and more number of users with higher individual utilities than the Nash equilibrium solution in most cases. The approaches for adjusting each users endowed monetary budget to improve the social utility and balance the individual utilities are also presented.

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## PP0

### Real Case Study - Application of a Memetic Algorithm for Scheduling in a Resins Production Plant (Using Parallel Reactors).

As operational changes are often, a memetic algorithm was developed for production scheduling to adapt to the news restrictions (for implemented restrictions). Three different and parallel reactors depend on the time of production of each resin and the gradual color increase. The weight function prioritizes others important dynamics situations, like v.i.p. customers, raw material prices, etc. The model was based on cluster structures population and heuristics to treat the restrictions.

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