Florian A. Potra:

Summary of Research (1994-2010)

The results of the research over the past 17 years are contained in 81 papers published in professional journals, and in 20 papers published in refereed proceedings. In what follows we summarize some of the main results.

Modeling atmospheric chemistry and air pollution

My interest in this area started at the "Center for Global and Regional Environmental Research" (CGRER) of the University of Iowa. There I worked in an interdisciplinary team together with Gregory Carmichael from the Chemical Engineering Department and several Ph.D. students in chemical engineering, computer science, and applied mathematics. The goal of that group was to develop a "Third Generation Model" for atmospheric chemistry. The requirements for such a model had been formulated by a panel of scientists (including Gregory Carmichael and myself) assembled by EPA [54]. It involved setting up a parabolic system consisting of about 300 nonlinear PDEs and finding efficient numerical methods for solving it. This is a 3-D reactive transport problem with about 100 chemical species and 200 chemical reactions. Since transport and chemical reactions operate at different time scales, an operator split technique is applied with different integration methods for transport and chemistry. In fact chemistry is solved by integrating at each point of the space grid a (very stiff) initial value ODE problem for a period of time equal to the time step of the transport integrator. Since up to 90% of computer time in atmospheric chemistry simulations is used in integrating chemistry, our group initially focussed its efforts on improving the chemistry integrators. This research effort lead to the reduction of the chemistry integration time by an order of magnitude and contributed to a better theoretical understanding of the behavior of numerical integrators for chemical rate equations.

The results of our research are contained in several papers ([24, 25, 26, 28, 39, 38, 93, 94, 97, 98, 99]). In order to easily test different chemistry models and different integration schemes, our group developed a symbolic preprocessor for chemical rate equations, KPP, which makes it very easy to build new chemistry models, automatically computes Jacobians, and determines a close to optimal reordering of chemical species in order to improve the sparsity of the LU factors to be used by implicit integrators. KPP is available on the Internet at htpp://people.cs.vt.edu/~asandu and has being used by many research teams around the world. A paper on KPP was published in [27].

Sensitivity analysis is another important aspect in modeling atmospheric chemistry. Estimating the sensitivity of the model with respect to initial conditions and parameters defining the model is crucial for interpreting the results and for model optimization. We proved that automatic differentiation can be a useful tool in computing sensitivities and we proposed a novel way of applying the software package ADIFOR to this effect [24, 25, 93, 94]. At present we are looking at efficient ways of building adjoint models for our problem. The use of automatic differentiation in the numerical solution of stiff ODEs is investigated in [36].

Simulating multibody systems

My research on multibody systems started at the "Center for Simulation and Design Optimization of Mechanical Systems" (CSDOMS) at the University of Iowa between 1987-1996, and at the "Center for Virtual Proving Ground Simulation: Mechanical and Electromechanical Systems" a Multi-University NSF-Army Industry/University Cooperative Research Center.

The first contributions are related to the numerical solution of mixed differential algebraic equations describing the governing equations of multibody systems. The papers [57, 59] describe how to properly implement multistep methods and Runge-Kutta methods for integrating such DAEs. The former paper is the written version of an invited plenary talk at the 1993 GAMM meeting in Dresden. In subsequent papers, we investigated various ways of improving the efficiency of DAE numerical integrators by appropriate use of sparse matrix techniques [52, 100]. In [9] we considered the role of outer inverses in multi-body system simulation. Papers [95, 96, 51] present a state-space based method for the numerical solution of the resulting DAEs. A subset of so called independent generalized coordinates, equal in number to the number of degrees of freedom of the mechanical system, is used to express the time evolution of the mechanical system. The second

order state-space ordinary differential equations (SSODE) that describe the time variation of independent coordinates are numerically integrated using a Rosenbrock type formula. For stiff mechanical systems, the proposed algorithm is shown to significantly reduce simulation times when compared to existent state of the art algorithms. The increased efficiency is due to the use of an L-stable integrator and the rigorous and general approach to providing analytical derivatives required by it. We mention that papers [96, 51] received the 2003 Professional Engineering Publishing Award of the Editorial Board of Journal of Multi-body Dynamics. Another algorithm for integrating index 3 DAEs specific to rigid multi-body dynamics, based on the Newmark formulae, is analyzed in [32]. The algorithm described in that paper was implemented by Dan Negrut in the MSC.ADAMS software package and has been successfully used for industrial strength dynamic analysis simulations.

My main area of interest has shifted to the simulation of multibody systems with contacts and friction. This is an active area of research with important applications in robotics (especially industrial assembly-line manipulators). Our results to date are collected in five papers [10, 11, 14, 16, 18]. It has been known for over one hundred years that there are examples of rigid multi-body systems with Coulomb friction that have no mathematical solution in the classical sense. Various authors have proposed different settings in which the rigid multi-body system problem with Coulomb friction has a generalized solution either by allowing for impulsive forces (i.e., a solution in the sense of distributions) or by considering the equations of motion as differential inclusions rather than differential equations. However, for the purpose of simulating multi-body systems with friction one needs a discrete model that has a computable solution. Paper [14] contains the first discrete model that has a computable solution under general conditions. A simulation package based on this model is being now implemented. The results obtained in [14] have earned my Ph.D. student Mihai Anitescu the prestigious James Wilkinson Postdoctoral Fellowship at Argonne National Laboratory. In a joint paper with Mihai Anitescu and David Stewart [18] we analyze the relationship between the discrete solution and the solution of the continuous problem in the sense of measure differential inclusions.

The time-stepping method proposed in [14] is not well suited to deal with stiff systems. Together with Mihai Anitescu [16] we managed to devise a time-stepping scheme that can efficiently handle such systems. We proved that for the most common type of stiff forces encountered in rigid body dynamics, where a damping or elastic force is applied between two points of the system, the method is well defined for any time step h. We show that the method is stable in the stiff limit, unconditionally with respect to the damping parameters, near the equilibrium points of the springs. The integration step approaches, in the stiff limit, the integration step for a system where the stiff forces have been replaced by the corresponding joint constraints. Additional properties of this scheme are given in [15]. Most of the time-stepping schemes from the literature that build a discrete model at a velocity-impulse level are based on Euler's method for solving ordinary differential equations (ODEs). In this context, the method of [14] is based on a semi-implicit Euler scheme, while the model of [17] is based on a linearly implicit Euler scheme. Both formulations require the solution of one linear complementarity problem (LCP) at each time step. In [71] we presented a new time-stepping scheme that uses a linearization of the modified trapezoidal method, incorporates a Poisson restitution model at collision, and solves only one LCP per time step when no collisions are encountered. We proved that under certain assumptions the method has order two, a fact that is demonstrated by our numerical simulations. To our knowledge this is the first superlinear time-stepping scheme for rigid multibody systems with contacts, joints and friction. For the case where the stiff forces originate in springs and dampers attached to points in the system, we use a special approximation of the Jacobian matrix which ensures that the LCP can be solved for any value of the parameters. Numerical simulations demonstrate that the method is stiffly stable. The method was implemented in UMBRA, an industrial-grade virtual prototyping software. UMBRA is marketed by Orion International Technologies of Albuquerque (`http://www.orionint.com/`) and is used in simulation studies at Sandia Labs. The Ageia company has built a physics engine for computer games called PhysX (`http://www.nvidia.com/object/physx_new.html`). They implemented one of our LCP-based time-steppers for multibody dynamics. They also designed the first PPU (physics processing unit) in order to boost performance, which is roughly 100 times the speed of competing systems.

In [33] we proved that the solution produced by a class of time-stepping schemes that solves one linear complementarity problem per step, and includes the methods presented in [14], [17] and [71] converges to a solution of a measure differential inclusion even when joint constraints are present. The main conceptual novelty is the reduced friction cone, which allows reducing the treatment of bilateral constraints to the

unilateral constraints case, without altering the pointedness property. In addition, we proved for the first time that certain trapezoid-like methods [71] converge in the sense of measure differential inclusions. In doing so, we were able to define a discrete velocity function of bounded variation, although the natural discrete velocity function produced by our algorithm may have unbounded variation.

When solving large-scale multibody dynamics, a relaxation of the standard (copositive) LCP formulation is desirable. In a recent paper [55] we have performed an extensive computational study using a convex relaxation introduced by Mihai Anitescu, which is convergent in the same weak sense described above. We have concluded that, by employing the interior point method from OOQP and the CHOLMOD linear algebra solver, it is possible to simulate in a robust manner very large multibody systems with contact and friction.

The work on multibody systems with contact and friction is likely to have a direct impact on several distinct engineering disciplines, including constrained mechanical systems with frictional contact arising in robotics and manufacturing. The need for discrete models of multibody systems with contact and friction was stressed at the "NSF Workshop on Mathematics and Robotics" that I organized in May 2001. The final report of that workshop can be found on my homepage www.math.umbc/~potra. In 2001 I was involved in consulting with Sandia National Laboratory on a project for developing a simulation environment for multibody systems with contact and friction. As a result of the cooperation with Jeff Trinkle, Vijay Kumar, Jong-Shi Pang, and David Stewart we have been awarded a Focused Research Grant from the National Science Foundation for: "Differential Algebraic Inequalities and their Applications in Engineering" (Grant No. 0139701 (2002-06)).

On March 4, 2010, I gave a MAA Distinguished Lecture entitled "Mathematics and Robotics", where I presented some open research problems in engineering, computer science, and mathematics, that need to be solved in order to fulfill the long standing promises of robotics
(`http://www.maa.org/dist-lecture/past-lectures.html`).

Interior point methods

In parallel with the interdisciplinary work described above, I have continued research on interior point methods. In a survey paper published in Optima (51, October 1996) Freund and Mizuno state that "Interior point methods in mathematical programming have been the largest and most dramatic area of research in optimization since the development of the simplex method... Interior point methods have permanently changed the landscape of mathematical programming theory, practice and computation...". While most of the research in this area was devoted to linear programming, in the opinion of the authors, "semidefinite programming is the most exciting development in mathematical programming in 1990s." For a more recent survey of interior point methods see [91].

During the 80's most papers on interior point methods concentrated on analyzing the computational complexity of different interior point methods for linear programming (LP) under the assumption that a strictly feasible point was given in advance. However this is hardly the case in practice. Theoretically, the difficulty may be overcome by a "phase I - phase II" approach, or via a "big M" approach, and the worst case complexity of the general problem is recovered. Practical algorithms, however, use starting points that lie in the interior of the region defined by the inequality constraints, but do not satisfy the equality constraints (for standard LP this simply means that the components of the starting point are positive). All subsequent points will have the same property, and, in the limit, optimal feasible solutions are obtained. The name infeasible-interior-point algorithm has been suggested to describe this type of method. Also, the best practical algorithms do not necessarily possess the best theoretical computational complexity. This is due to the limitations of the worst case analysis used in deriving polynomial complexity bounds and reflects the inherent conflict between the requirements of global convergence and fast local convergence. In an attempt to address both paradigms mentioned above I proposed in [56] the first infeasible-interior-point algorithm having both polynomial complexity and superlinear convergence. This result was generalized for linear complementarity problems (LCP) in [61]. A simplified version of the algorithm was given in [101].

The vast majority of papers on interior-point algorithms study only the convergence of the complementarity measure $(x^k)^T s^k$, but not the convergence of the iteration sequence $\{x^k, s^k\}$ produced by the algorithm. In [20], sufficient conditions are given for a class of infeasible–interior–point algorithms to produce convergent iteration sequences. An efficient algorithm of this type is analyzed in [31]. In [62], I gave rather general sufficient conditions under which the iteration sequence is Q-quadratically convergent, and I showed that these conditions are satisfied by several well known interior-point methods. In particular it follows that the

iteration sequences produced by the simplified predictor–corrector method of Gonzaga and Tapia, the simplified largest step method of Gonzaga and Bonnans, the LPF+ algorithm of Wright, the higher order methods of Wright and Zhang, Potra and Sheng, and Stoer, Wechs and Mizuno are Q-superlinearly convergent, a fact that had not been previously known.

Superlinear convergence of interior-point-methods for LCP is proved under the assumption that the problem is non-degenerate in the sense that it has a strictly complementary solution. In fact, according to a result of Monteiro and Wright, standard interior-point-methods cannot be superlinearly convergent for degenerate problems. While any LP has a strictly complementary solution, this is not the case with many important LCPs. Therefore, for such problems it is important to find either acceleration procedures or efficient finite termination schemes. In [40] the convergence of the Tapia indicators for infeasible–interior–point methods for solving degenerate linear complementarity problems is investigated, and a finite termination procedure is proposed. A nonstandard infeasible–infeasible–interior–point method that is superlinearly convergent for degenerate LCP is proposed and analyzed in [82]. I have also analyzed a predictor-corrector method for linear complementarity problems acting in a larger neighborhood of the central path that has $O(\sqrt{n})$-iteration complexity under general assumptions, and quadratic convergence under the strict complementarity assumption [63].

In [44, 41, 78, 79] these results are further refined and generalized for the P_*-matrix LCP. Other results on interior-point-methods for linear and nonlinear programming are contained in [13, 12, 35, 43, 60, 92, 66].

The best computational complexity results for the linear complementarity problem (LCP) have been obtained by using interior point methods that act in a small (i.e., l_2) neighborhood of the central path. The same is true for the particular case of linear programming (LP). The best computational results to date show that such interior point methods can solve the problem in $O(\sqrt{n}L)$ iterations, where n is the dimension of the problem and L is the bit-length of the data. However, practical algorithm act in a large neighborhood (i.e., l_∞) of the central path. In spite of their practical efficiency, the theoretical computational complexity results obtained until recently in the literature for such algorithms were much worse than for interior point methods based on small neighborhoods of the central path. In 1999 Gonzaga has managed to show that a predictor-corrector method based on a large neighborhood of the central path has $O(nL)$-iteration complexity, the same as the best complexity achieved at that time by any other known interior-point method in this neighborhood that uses only first order derivatives.

In [64] we proposed a new predictor-corrector interior point method for monotone LCPs acting in a wide neighborhood of the central path. Given a point z in a wide neighborhood of the central path, $z \in \mathcal{N}_\infty^-(\alpha)$, the algorithm uses a higher order predictor to compute a point $\bar{z}$ in a slightly larger neighborhood of the central path $\bar{z} \in \mathcal{N}_\infty^-(\alpha+\gamma)$, $\gamma = \alpha(1-\alpha)/(n+1)$. Then, by applying a first order corrector at $\bar{z}$, the algorithm computes a point $z^+ \in \mathcal{N}_\infty^-(\alpha)$, so that the predictor-corrector scheme can be iterated. The method has $O(\sqrt{n}L)$-iteration complexity and is superlinearly convergent even when the problem does not possess a strictly complementary solution.

The above algorithm was improved in [67]. The improved algorithm is presented as a corrector-predictor method rather than a predictor-corrector method. In this variant one starts with a point in $\mathcal{N}_\infty^-(\alpha)$, and one uses a corrector to produce a point closer to the central path, followed by a predictor step to obtain a point on the boundary of $\mathcal{N}_\infty^-(\alpha)$. The advantage of this approach is that only one neighborhood of the central path needs to be considered, avoiding thus the explicit relation between the "radii" of the two neighborhoods reflected in the choice of the quantity γ from the paragraph above. It turns out that one could get rid of the corrector step altogether, if one increases the radius of the wide neighborhood at each iteration. Indeed, in [68] we have shown that by using a higher order affine scaling direction, and by enlarging the neighborhood at each iteration, it is possible to obtain an interior point method with $O(\sqrt{n}L)$-iteration complexity and superlinear convergence even in the absence of strict complementarity.

The predictor-corrector method from [64] was generalized in [72] for sufficient LCPs. The straightforward generalization again uses two neighborhoods of the central path $\mathcal{N}_\infty^-(\alpha) \subset \mathcal{N}_\infty^-(\alpha+\gamma)$. The algorithm works if $\gamma = \alpha(1-\alpha)/(n(1+4\kappa)+1)$, where κ is the handicap of the sufficient LCP, i.e. the smallest number for which the LCP is $P_*(\kappa)$. In this case, however, the algorithm would depend on the handicap κ which is usually unknown. An interior point method that does not depend explicitly on κ is obtained by starting with a guess for κ and then doubling κ in those iterations where a certain test fails. The resulting algorithm has $O((1+\kappa)\sqrt{n}L)$ and is superlinearly convergent even for degenerate LCPs. These difficulties are alleviated

in [47] where one extends the algorithm from [67] for sufficient LCPs. Since that algorithm is a corrector-predictor method it uses only one neighborhood $\mathcal{N}_\infty^-(\alpha)$, where α can be any number in the interval $(0,1)$ and therefore it does not depend on the handicap of the sufficient LCP. In [65] we showed that the use of Kantorovich's theorem from nonlinear analysis leads to a better understanding of the behavior of interior point methods. The complexity results presented above are proved that a strictly feasible starting point is available. An infeasible start corrector-predictor method for sufficient LCP is analyzed in [37]

The practical performance of a numerical algorithm is better explained by a probabilistic complexity analysis rather than by a worst case complexity analysis. For example the practical performance of the simplex algorithm is much better characterized by its probabilistic computational complexity (which is strongly polynomial) than by its worst case complexity which is exponential. The state of the art worst case complexity results for interior point methods show that a standard linear program with integer data of bit-length L can be solved in $O(\sqrt{n}L)$ steps, where n is the dimension of the problem. Each step involves at most $O(n^3)$ arithmetic operations, so that the worst case computational complexity of interior point methods is linear in L and polynomial in n. Since the computational complexity depends on the bithlength of the data the interior point methods are "weakly" or "pseudo" polynomial. In [19] we showed that from a probabilistic point of view the complexity of interior–point–methods for linear programming can be reduced to $O(\sqrt{n}\ln n)$. This result holds both as a high probability result and expected value, and shows that the probabilistic computational complexity of interior–point methods is strongly polynomial. In [42] we considered the problem of finding an $\epsilon-$optimal solution of a standard linear program with real data, i.e., of finding a feasible point at which the objective function value differs by at most ϵ from the optimal value. In the worst-case scenario the best complexity result to date guarantees that such a point is obtained in at most $O(\sqrt{n} \mid \ln\epsilon \mid)$ steps of an interior point method. We showed that the expected value of the number of steps required to obtain an $\epsilon-$optimal solution for a probabilistic linear programming model is at most $O(\min\{n^{1.5}, m\sqrt{n}\ln(n)\}) + \log_2(\mid \ln\epsilon \mid)$.

Semidefinite programming (SDP) consists in minimizing a linear functional of a matrix subject to linear equality and inequality constraints, the inequality constraints being understood in the sense of the cone of positive semidefinite matrices. SDP contains LP and convex quadratic programming (QP) as particular cases. Also, SDP has important applications in such areas as control and system theory, structural optimization, pattern recognition, and statistics. Lately, semidefinite relaxations of NP-hard problems have been found, that provide very good approximation algorithms. For example, Goemans and Williamson showed that the optimal value of a semidefinite programming problem is at most 14% above the value the MAX-CUT problem.

While LP and linearly constrained QP can also be solved by other methods, (e.g. Simplex or Lemke) interior point methods appear to be the only methods that can efficiently solve SDP. The design and analysis of interior point methods for SDP is considerably more complicated than for LP or QP.

In [83] we analyzed a generalization of the Mizuno-Todd-Ye predictor–corrector method for SDP. The iteration complexity depends on the quality of the starting point. If the problem has a solution, then the algorithm is globally convergent. If the starting point is feasible or close to being feasible, the algorithms finds an optimal solution in at most $O(\sqrt{n}L)$ iterations. If the starting point is large enough, then the algorithm terminates in at most $O(nL)$ steps, either by finding a strictly complementary solution, or by determining that the primal-dual problem has no solution of norm less than a given number.

Superlinear convergence is especially important for SDP, since no finite termination schemes exist for such problems. As predicted by theory and confirmed by numerical experiments, the linear systems defining the search directions become very ill conditioned as we approach the solution. Therefore an interior-point method that is not superlinearly convergent is unlikely to obtain high accuracy in practice. The first superlinear convergence results for interior point methods for SDP were obtained in [83]. The results of the latter paper were improved in [81] and generalized in [45], [46]. The algorithm considered in [84] was the first algorithm for SDP with polynomial complexity and superlinear convergence without imposing shrinking of the central path neighborhood used for determining the step-length.

Normally, the search directions used by interior point methods for SDP are symmetric. However, in some cases it may be more efficient to use non-symmetric search directions. The first study of such directions was done in [22].

Practical experiments show that the performance of the interior point algorithms for SDP deteriorates

if the algorithms are started from infeasible points. To alleviate this problem we proposed in [80] a simple homogeneous primal-dual feasibility model for semidefinite programming problems. We considered two infeasible–interior–point algorithms for solving the homogeneous formulation. The algorithms do not need big M initialization. If the original SDP problem has a solution, then both algorithms find an ϵ-approximate solution (i.e., a solution with residual error less than or equal to ϵ) in at most $O(\sqrt{n}\ln(\rho^*\epsilon_0/\epsilon))$ steps, where ρ^* is the trace norm of a solution, and ϵ_0 is the residual error at the (normalized) starting point. A simple way of monitoring possible infeasibility of the original SDP problem is provided, so that in at most $O(\sqrt{n}\ln(\rho\epsilon_0/\epsilon))$ steps either an ϵ-approximate solution is obtained, or it is determined that there is no solution with trace norm less than or equal to a given number $\rho > 0$. Numerical experiments showed superior performance of these algorithms both for feasible and infeasible problems.

We have implemented in *Mathematica* twelve interior-point methods for SDP. Numerical results show that the homogeneous algorithms generally have better performance than their corresponding non-homogeneous versions. The package SDPHA and some numerical results are described in the report [21]. We have also developed a MATLAB package [23] and we are presently working on a C++ code capable of solving large scale semi-definite programming problems.

A variable precision variant of SDPHA, called SDPHA6, implemented in *Mathematica 6*, was used for computing optimally conditioned positive definite Hankel matrices of order n. Unlike previous approaches, our method is guaranteed to find an optimally conditioned positive definite Hankel matrix within any desired tolerance. Since the condition number of such matrices grows exponentially with n, this is a very good test problem for checking the numerical accuracy of semidefinite programming solvers. Our tests show that semidefinite programming solvers using fixed double precision arithmetic are not able to solve problems with $n > 30$. Moreover, the accuracy of the results for $24 \leq n \leq 30$ is questionable. By using the variable precision code SDPHA, we have validated the results obtained by standard codes for $n \leq 24$, and we have found optimally conditioned positive definite Hankel matrices up to $n = 100$ [1].

In [69] we have considered a path following interior point method for solving linear complementarity problems over symmetric cones. We mention that cone of semidefinite matrices and the cone of positive vectors are particular cases of symmetric cones. The starting point of our our algorithm has to be strictly feasible with respect to the inequality constraints, but may be infeasible with respect to the equality constraints. Therefore the algorithm falls in the broad class of infeasible interior point methods. The algorithm is a corrector-predictor type method that generalizes several corrector-predictor methods presented in the literature. It has polynomial complexity under general assumption and superlinear convergence under some mild additional assumptions.

Our research on interior point method has been supported by several NSF grants, including "Interior Point Methods for Complementarity Problems", Grant No. 0728878 (2007-2010).

Numerical optimization methods, and in particular interior point methods, have numerous applications in science and engineering. For several years, I have been a consultant with the United Technologies Research Center on several such applications. This activity resulted in patent (James W. Fuller , Indraneel Das , Florian Potra and Jun Ji : SYSTEM AND METHOD OF APPLYING INTERIOR POINT METHOD FOR ONLINE MODEL PREDICTIVE CONTROL, Serial Number 11 / 150 , 703 Filed in the United States of America on June 10 , 2005).

Solving nonlinear equations

I have also continued, albeit less intensely, research on the numerical solution of nonlinear equations. In [3] (see also [2]) we used the Kantorovich convergence analysis combined with interval arithmetic techniques to obtain an efficient validation procedure for the numerical solutions of nonlinear systems. The ideas from this paper were applied to validate solutions of linear complementarity problems in [6], and of nonlinear complementarity problems in [7]. It is interesting to note that the Kantorovich convergence analysis can be effectively used in the convergence analysis of interior point methods for linear complementarity problems [65]. Also, in a related paper, we analyzed the relationship between the theorems of Kantorovich, Moore and Miranda [8].

We proposed and implemented a new nonlinear solver that is more efficient on some classes of problems than the standard solvers [4]. Finally, we analyzed some new secant methods for solving nonlinear systems of semismooth equations [77]. Since nonlinear complementarity problems can be written as nonlinear systems

of semismooth equations, the methods described in [77] could be used as an alternative solution method. Other results belonging to this general field are contained in [2, 5, 58, 85, 86].

Bioinformatics

This is a new area of research for me, but one into which I have put a lot of effort over the past several of years within the Bioinformatics Research Center at UMBC. Our research in this area was supported by the National Institute of Health (Grant No. R01GM075298-01 (2005–09)).

In [75] we presented several algorithms with polynomial complexity for separating two sets of points in the n-dimensional space that have nondisjoint convex closures. The algorithms are used in a supervised machine learning framework to predict the likelihood of a patient having malignant breast cancer tumors by comparing the patient's 9 attributes (Clump Thickness, Uniformity of Cell Size, Uniformity of Cell Shape, Marginal Adhesion, Single Epithelial Cell Size, Bare Nuclei, Bland Chromatin, Normal Nucleoli, and Mitosis) with similar data in existing cancer databases. We have also tested our methods on the Wisconsin Diagnostic Breast Cancer data set, where 30 attributes are associated with each patient.

In [76] we proposed new registration methods for 2D-electrophoresis gels with application in proteomics. The proteome analysis involves the separation, visualization, and analysis of complex mixtures containing as many as several thousand proteins obtained from whole cells, tissues, or organisms. Two dimensional polyacrylamide gel electrophoresis (2D-PAGE) is the core technology for separating complex protein mixtures in the majority of proteome projects. Due to the complexity of the 2D-PAGE procedure, gel-to-gel experimental variation is huge. Even under strictly controlled laboratory conditions, the same sample can yield quite different protein maps in different runs. A spot that appears at one location on a given image may appear at a very different location on another image. The algorithms developed in our paper provide tools for better image alignment for spot matching and for constructing a master gel representing the subject, which facilitates detection of the biological variation and the variation attributed to treatment effect or exogenous stimulus like environmental changes.

In order to overcome the shortcomings of both forward and inverse transformations, we proposed a new approach for aligning families of 2D-gels. First, the locations of the ideal landmarks on the ideal gel, along with the approximate size of the ideal gel, are obtained as the solution of a large scale quadratic optimization problem. The quadratic programming problem can be efficiently solved by interior-point methods even for large families of gels. In the forward phase of the method, a relatively coarse grid is used. Inverse transformations are then constructed for each source gel by using a sequence of finer grids, which results in an improved alignment of the family. Both the forward and the inverse transformations are constructed in such a way that they are very likely to be one-to-one mappings. Moreover, because the domain considered in the inverse transformations is in the range of the forward transformations, there will be no pixels beyond the range of the inverse transformation. After obtaining the inverse transformation, intensities cam easily be assigned for all the pixels of the transformed source images, and the transformed images are well aligned. This new paradigm was implemented by using piecewise bilinear transformations on a hierarchical grid as well as tensor product cubic splines. By using the new algorithm it was possible, for the first time, to simultaneously align families of 2-D gels containing over 100 gels. The results are contained in the papers [73, 74]. A theoretical framework for analyzing the protein image alignment algorithms is presented in [70]

Multi-hazard Structural Design

The objective of multi-hazard structural engineering is to develop methodologies for achieving designs that are safe and cost-effective under multiple hazards. In a series of joint papers with Emil Simiu [87, 88, 89] we formulated the multi-hazard structural design problem in nonlinear programming terms, and analyzed the difficulties of its numerical solution. In [89] we presented a simple illustrative example involving four design variables and two hazards: earthquake and strong winds. The results of our numerical experiments showed that interior-point methods are significantly more efficient than classical optimization methods in solving the nonlinear programming problem associated with this example.

It is important to note that the design variables should be determined is such a way that the load-induced stresses and deflections are kept below specified thresholds at all points of the resulting structure. Since there are infinitely many such points, the optimization problem becomes a semi-infinite programming problem. In [88] we discussed the difficulties involved in the numerical solution of the semi-infinite programming problems arising in multi-hazard structural design. We showed that it is possible to construct efficient and

robust optimization algorithms, by adaptively choosing a family of finite sets of points on the structure, and by using interior point methods for solving the corresponding nonlinear programming problems.

Miscellaneous

Paper [90] deals with some low order methods for solving singular integral equations. In [50, 49] new algorithms are proposed for signal-adapted QMF bank design. In performing on-board Model Predictive Control of dynamical systems, it is necessary to solve a sequence of optimization problems (typically quadratic programs) in real-time to generate the best trajectory. Since only a low fixed number of iterations can be executed in real time, it is not possible to solve each quadratic program to optimality. However numerical experiments show that if we use information from the numerical solution of the previous quadratic program to construct a warm start for the current quadratic program, there is a time step after which the usual stopping criteria will be satisfied within the fixed number of iterations for all subsequent optimization problems. This phenomenon, called subsequent convergence is analyzed in [29]. In [53] we made some connections between flow invariance, first and second order tangent cones, and nonlinear programming. The paper [34] is concerned with presenting a method for the analysis of delay differential equations with periodic coefficients through the use of an integral representation of the monodromy operator. A collocation procedure is used to approximate the fundamental solution, and the eigenvalues of the discretized monodromy operator are shown to converge to the eigenvalues of the integral operator. This allows the stability of the equation to be analyzed. The research in [34] was motivated by an application to machining. A survey paper on smart machining systems was published in [30]. In [48] we proposed a two-stage stochastic second-order cone programming formulation of the semidefinite stochastic location-aided routing (SLAR) model in mobile ad hoc networks. The aim of SLAR is to provide a sender node S, with an algorithm for optimally determining a region that is expected to contain a destination node D (the expected zone). The movements of the destination node are represented by ellipsoid scenarios, randomly generated by uniform and normal distributions in a neighborhood of the starting position of the destination node. By using a second-order cone model, we were able to solve problems with a much larger number of scenarios (20250) than it is possible with the semidefinite model (500). The use of a large number of scenarios, allows for the computation of a new expected zone, that may be very effective in practical applications, and for obtaining stability results for the optimal first-stage solutions and for the optimal cost function values.

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