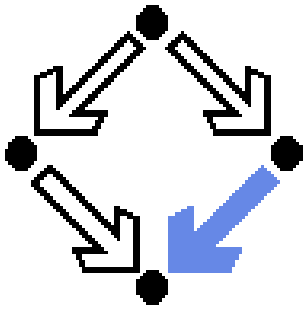

Abstract Booklet

Conference
Symbolic and Numerical
Scientific Computation

(SNSC'01)

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Research Institute for Symbolic Computation
Schloss Hagenberg, Austria

Symbolic computation of series and products using zeta regularization technique

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In this talk I will discuss zeta regularization of divergent series and its application to symbolic computation of infinite products. For example,

$$\lim_{N\to\infty} \prod_{n=1}^{2N} \left(1+\frac{1}{n}\right)^{-n(-1)^n} = \frac{A^6}{2^{\frac{1}{6}}\, e\, \sqrt{\pi}}$$

where A is Glaisher-Kinkelin's constant. I also apply this technique to computation of determinants of the Laplacian. The multiple Barnes function, defined as a generalization of the Euler gamma function, naturally appeared on this path as the essential part of this formalism.

Passive Complete Orthonomic Systems of PDEs and Riquier Bases of Polynomial Modules

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The object of this talk is to enlighten the relationship between the two classical theories of passive complete orthonomic systems of partial differential equations (PDEs) at the one hand side and of Gröbner bases of finitely generated modules over polynomial rings at the other hand side. The link between both types of canonical forms are the Riquier bases (also called 'involutive bases' in the literature) which are at the same time a particular type of Gröbner bases carrying some additional structure and a natural translation of the notion of passive complete orthonomic systems of PDEs into the language of polynomial modules.

We will point out some desirable applications which a "good" notion of Riquier bases could provide. In particular, we will consider a theoretical application in combinatorial algebra which shows that the importance of Riquier bases is not restricted to only the vague hope to design a new faster algorithm for computing Gröbner bases. Unfortunately, the requirements arising in different applications turn out to partially collide which leads us to the discussion on finding a reasonable compromise.

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Exact Distribution of Estimators of Parameters in AR(1) Processes by the Help of MAPLE

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Let us consider the stochastic differential equation

$$d\xi(t) = -\lambda\xi(t)dt + \sigma_w dw(t), \qquad \sigma_w > 0,$$

where w is a standard Wiener process. $\xi(t)$ is called an Ornstein-Uhlenbeck or AR(1) process [1].

In the theory of diffusion processes, λ is called the drift parameter, but in the theory of ordinary differential equations it is called the damping (or decay) parameter.

The exact distribution of the maximum-likelihood estimator of the drift (damping) parameter in a stationary AR(1) (or Ornstein-Uhlenbeck) process is investigated [2]. Quantiles of the distribution function for different levels are given.

The main goal is to reproduce, by the help of PC and MAPLE, the table of the distribution function of maximum-likelihood estimator, given by Prof. Arató, and calculated on URAL and CDC 3300 computers.

When we reproduced the earlier calculations, the applied hardware was a SUN Sparc Station with operating system SUN OS. The software tool was the MAPLE, Release 2, which can be efficiently used for symbolical and numerical computations.

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A Symbolic Procedure for the Diagonalization of Linear PDEs in Accelerated Computational Engineering

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Since early 90's in the past century our research has been focused on the acceleration of computer simulations of PDEs. Another equally important and uncompromising objective has been the accuracy enhancement of the numerical results. As a first step towards these goals we have devised a symbolic procedure for systematically and conveniently diagonalizing the linear PDEs, which are commonly encountered in mathematical physics and computational engineering applications.

This presentation provides a detailed account of the ideas behind diagonalization, and discusses its consequences on designing robust, accurate and accelerated algorithms for solving boundary value problems (BVPs) in both integral- and differential form.

The discussion starts with a conjecture stating that *all linearized PDEs, as models for physically realizable systems, can be diagonalized.* As byproducts, our conjecture implies several constraints, consistent with known classical results, upon the involved constitutive equations.

Diagonalized forms are, by construction, equivalent to the originating PDEs, but distinguish the space coordinate with respect to which the diagonalization has been performed. As will be shown in this presentation diagonalized forms intrinsically allow several useful interpretations which are generally deeply hidden in their PDE counterparts.

We demonstrate the technical details by converting several PDEs into their respective diagonalized forms. In particular we consider the Laplace equation for the electrostatic and magnetostatic fields, elastostatic equations, the Helmholz equation for the scalar wave propagation, the acoustic-, piezoelectric-, and electromagnetic wave equations for vector fields in anisotropic and transversally inhomogeneous media, and finally the Schrödinger wave equation. Thereby, a symbolic notation, which can easily be automated, will enable us to replace lengthy and tedious calculations by a *simply-by-inspection* manipulatory procedure.

For reasons which will be made clear we refer to diagonalized representations as Huygens' Principle in Differential Form. We will interpret this principle and show that it can favorably be used for (i) generating novel stencils in the finite difference method (leading to our recently developed *Differential Boundary Element Method, DBEM*); (ii) constructing functionals in the finite element method; and most importantly, (iii) establishing singular surface integrals in the boundary element method.

Diagonalized forms in spectral domain transform into algebraic eigenvalue equations. Using the associated eigenpairs we suggest three procedures for constructing Green's functions associated with a given boundary value problem, keeping in mind the automatization aspect in our derivations.

We investigate the asymptotic properties of the eigenpairs in the far- and near-field in the spectral domain. In accordance with Heisenberg's uncertainty principle these asymptotic expansions correspond to the near- and far-fields in the spatial domain. Utilizing the far-field expansions in the spectral domain we propose an easy-to-implement recipie for the regularization of singular surface integrals in the boundary element formulations. For completeness, the presentation of the proposed regularization will proceed a discussion on Hadamard's definition of well-behavedness of linear operator equations, and Tikhonov's regularization technique.

Using our regularization technique we show that moments of Green's functions associated with a given BVP can be written in coordinate (geometry)-free, frequency-, and material independent forms, and therefore, they can be regarded as *universal functions* for the underlying class of problems. It turns out that the universal functions are generally astonishingly smooth; they can be precalculated, stored, and thus retrieved as often as required (data recycling). This capability allows us to separate the scientific computing efforts from the pre- and postprocessing steps in simulations, suggesting the following organization of our software: preprocessing-buffer-computational:engine-buffer-postprocessing. These considerations have resulted in the development of the Fast-MoM, which is an accelerated form of the conventional method of moments (boundary element method).

Using precalculated universal functions the computation times for the calculation of *impedance matrices* in the BEM applications reduce to the times required for retrieving data from the chosen storage medium. However, in spite of this advancement, a major drawback in the BEM still remains to be removed: the impedance matrices are dense. Several techniques have been suggested in literature for obtaining sparse matrices, each with its own limitation. We have suggested a procedure which consists of constructing problem-specific orthogonal sequences of basis functions derived from the involved Green's functions. The idea is to expand the unknowns in our problems in terms of basis functions which embed intrinsic features of the underlying PDEs in their structures: Using Meyer's orthogonalization technique and Green's functions associated with a given BVP, we construct functions which are orthonormal to their integer-translates. In the case of Laplace operator, we are able to show that the resulting functions even support a multiresolution analysis, leading to *Green's-functions-based scaling functions and wavelets*. Several numerical examples will illuminate the underlying concepts.

We continue our presentation by briefly discussing several alternative *localization* techniques for generating sparse matrices in computations, including coherent states and Wannier fucntions, originally suggested in quantum mechanics, and photonics applications, respectively.

We conclude our discussion by posing the following *existence* question: Why is it possible to diagonalize a given system of linearized PDEs in the first place?

Accurate Numerical Fourier Transform in d-Dimensions.

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April 11, 2001.

ABSTRACT. The classical method of numerically computing Fourier transforms of digitized functions in one or in d-dimensions is the so-called *Discrete Fourier Transform* (DFT) efficiently implemented as *Fast Fourier Transform* (FFT) algorithms. In many cases, the DFT is not an adequate approximation of the continuous Fourier transform. Because the DFT is periodical, spectrum aliasing may occur. The method presented in this contribution provides accurate approximations of the continuous Fourier transform with similar time complexity. The assumption of signal periodicity is no longer posed and allows to compute numerical Fourier transforms in a broader domain of frequency than the usual half-period of the DFT. The aliasing introduced by periodicity can be reduced to a negligible level even with a relatively low number of sampled data points. In addition, this method yields accurate numerical derivatives of any order and polynomial splines of any odd order with their optimum boundary conditions. The numerical error on results is easily estimated. The method is developed in one and in d-dimensions and numerical examples are presented.

Multivariate polynomials and Newton-Puiseux expansions

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In this paper, we will be interested in the local resolution of equations of the type:

$$f(y) = 0 \text{ with } f \in \mathbb{C}[x_1, \ldots x_N, y]$$

To express the solutions, we will need a generalization for several variables of the Puiseux series: the series with exponents in a cone. To compute these series, we use an extension of the classical Newton polygon, the Newton polyhedron.
After a first part, in which we give some definitions and properties about elements of convex geometry and series with exponents in a cone, we present a resolution algorithm due to J. McDonald. We will take his work as starting point for the resolution process and improve it to obtain an algorithm computing what we called a full set of solutions. That is to say a set of couples composed of a cone and the associated series expansions of the solutions. More precisely, we consider the discriminant of f, with respect to the variable y, and the fan of its Newton polyhedron. To each cone σ of this fan, we can associate pathes of the Newton polyhedron of f and solutions expansions with exponents in a translate of σ.
For example, for the equation:

$$f(x_1, x_2, y) = x_2y^2 + y^2 + x_2^2y + x_1^2y + x_1^2x_2y - x_1x_2$$

we find three cones and for each cone we compute two solutions.

Exact Real Computation in Computer Algebra*

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Abstract

This talk describes our approach to represent computable real numbers in Maple. We aim at a model that can be used in symbolic computation.

The main topics we discuss are: representation and arithmetic of exact real numbers, vectors and matrices; polynomial arithmetic and root computation. Some operations raise ill-posed problems; we used regularization methods to solve them.

1 Extended Abstract

Many algorithms in symbolic and algebraic computation rely on exactness. The usual way is to work with the subfield of rationals or real algebraic numbers; the later are traditionally represented by the minimal polynomial and either an isolated interval or a sequence of signs [7]. It is sometimes a problem that these subfields are not closed under transcendental functions such as exponentiation or trigonometric functions. Even if we stay within algebraic operations only, it turns out that the manipulation of real algebraic numbers is very expensive [10].

The method of *exact real computation* seems to be a reasonable alternative: it provides a *a mathematically consistent representation* of the represented reals, as the models behave exactly like the mathematical objects which they represent. Recall that this is not the case for floating point numbers, and this is one of the reasons why working with floating point numbers is so often difficult in computer algebra.

Several ways to represent the reals have already been invented; we mention here infinite (lazy) strings of digits ([6], with golden ratio notation, [9], [5]) and a functional approach, where the reals are represented as functions that produce approximations on demand [3].

Our approach is more pragmatically oriented towards the usability within computer algebra. Of course, efficiency of the arithmetic has been an issue, but our intention was not to invent a new arithmetic that could compete with the fastest existing ones. Instead, we took an objectual approach, which makes it easy to change the details in the representation at the lowest level independently of the higher level algorithms. It may be remarked that this has already paid off, as we were already forced to change details on the low level at a state where a lot of higher algorithms already existed.

A general performance problem in computer algebra is the one of *intermediate expression swell*. We still have it when using exact real computation, but much more moderate: in symbolic-exact arithmetic, the expressions may grow exponentially with the number of arithmetic operations (e.g. minimal polynomials under addition and multiplication of algebraic numbers, or mantissa lengths under powering of rational numbers). But in exact real computation we can always achieve linear growth. The size of a result is always equal to the size of the arguments plus a constant overhead for the operation itself. On the other hand, it has to be remarked that intermediate simplification (e.g. canceling) does not occur in exact real computation.

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We utilize the fact that most existing computer algebra systems already have a built-in arbitrary precision arithmetic and conversion algorithms between numerical and symbolic data. For many problems, it suffices to supply small wrappers which encode the necessary information about the error propagation. Sometimes this information is already available in the literature of numerical analysis (see e.g. [8]). An example is our algorithms for computing roots of squarefree polynomials (section 4.3).

However, there are other problems which lead to fundamental difficulties because their solution does not depend continuously on the input data: *pseudo-inverse of rank-deficient matrices, polynomial greatest common divisor (gcd) computation, multivariate polynomial factorization, curve and surface parameterization.* Strictly speaking, these problems cannot be solved within exact real computation (see [1]). As we definitely need a substitute for these ill-posed problems, we apply the common technique of *regularization*: we replace the problem by a nearby continuous problem (the distance to the exact problem is an additional input parameter). We apply Tikhonov regularization [2] (see also [4]) to the computation of pseudo-inverses and gcd's.

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Database of graded rings and K3 surfaces in Magma

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K3 surfaces are one of the kinds of algebraic surface which naturally generalise elliptic curves. They are also very closely related to canonical models of curves and lie right in the heart of the classification of surfaces. Elliptic curves can be expressed in various standard formats: a plane cubic in Weierstrass form, an intersection of two quadrics in space, and so on. The standard first example of a K3 surface is defined by a homogeneous degree 4 polynomial in 4 variables (compare that with degree 3 in 3 variables for an elliptic curve). But there are very many other K3 surfaces in interesting formats.

I will report on a database of K3 surfaces in the computer algebra system Magma. This is built using Hilbert series methods which describe the degrees of variables and equations in some graded ring. The methods generate candidates for K3 surfaces which one must then show actually exist with the desired properties. The most interesting aspect of this is the way in which the inductive construction of the database helps to prove the existence of the objects which it contains.

I will show examples of K3 surfaces and give a description of the Hilbert series methods used to find candidates. Then I will indicate how the method of "unprojection" in conjunction with the building of the database can show the existence of these rather complicated graded rings. This is joint work with Selma Altınok and Miles Reid.

TH∃OREM∀: A System for the Working Mathematician

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The main goal of the TH∃OREM∀ project[1] is to deliver an integrated interactive environment which can assist the mathematician in all the phases of his scientific work: proving, computing and solving in various mathematical domains. The system is implemented on top of *Mathematica*, thus it is backed by the full algorithmic and computing power of the currently most popular computer algebra system, which is available on all the main computing platforms (Unix, Linux, Windows, and Apple). The current implementation is the result of several man-years of work by many people of the TH∃OREM∀ group at RISC (see `www.theorema.org`), under the direction of Bruno Buchberger. Until now, we already built into the system the main features concerning *proving* and *computing*, while the *solving* features are in the design phase. The main features of the system will be demonstrated live during this presentation.

The system interacts with the user in the language of *predicate logic*, which is the natural language for expressing mathematical properties and algorithms. Few intuitive commands allow the user to enter mathematical formulae (in natural two-dimensional notation) and to compose them into mathematical theories, and also to use some basic domains (numbers, tuples, sets) which are already provided in TH∃OREM∀. Moreover, the system provides the implementation of the powerfull concept of *functor*, which allows the build-up of sophisticated domains on top of simpler ones. The mathematician has the possibility to experiment with the algorithms expressed in this way by directly running them using the TH∃OREM∀ *computing* engine, and he can also study their formal properties (e.g. correctness) using the *provers* of TH∃OREM∀. It is an unique feature of TH∃OREM∀ that these two phases of the mathematical activity can be performed in the *same integrated system* and using the *same language*.

Computation is performed under full control of the user, which means being able to trace the reason (definition, formula) for each computing step – if necessary, but most important with full control of the *knowledge* which is used in the computing process. For instance, in a certain situation the mathematician wants to give to the symbols **, +, 0, Successor* the axiomatic meaning as defined by induction over natural numbers, while in another situation the same symbols should be interpreted using the full power of the underlying computational engine (positional notation, long arithmetic, etc.)

Proving is done with specific methods for several mathematical domains: propositional logic, general predicate logic, induction over integers and over lists, set theory, boolean combinations of polynomial [in]equalities (using Groebner Bases), combinatorial summation (using Paule–Schorn–Zeilberger), and a novel technique for proving in higher-order logic with equality: PCS (proving–computing–solving), introduced by Buchberger. TH∃OREM∀ departs from the methods mostly used in automatic provers today, because it uses a *natural proving style*: the formulae are expressed in their original form (two-dimensional, non-clausal), the inference steps are expressed in natural style and in human language, and – most importantly – the proving methods are similar to the ones which are used by the working mathematicians. Therefore, the user has the possibility to inspect and easily understand the proofs, to verify any inference, and to interact with the proof by modifying certain assumptions, etc.

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A progress report on formalizing theory of commutative ring

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The elementary properties of rings and ideals in the chapter one of Atiyah and MacDonaldc's book "introduction to commutative algebra" is formalized in Isabelle HOL. We present the details of definitions, theorems and proofs related rings and ideals in Isabelle.

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Set-Oriented Numerical Methods for Dynamical Systems

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Over the past few years so-called set-oriented numerical methods have been developed for the numerical study of dynamical systems. These methods do not just allow to compute *directly* – i.e. by avoiding long term simulations of the underlying system – invariant sets or invariant manifolds but they can also be used to approximate statistical quantities such as natural invariant measures. In this talk an overview about recent accomplishments in this area will be given. In particular, three concrete applications of these techniques will be presented: the approximation of so-called *almost invariant sets*, the construction of reliable global zero finding procedures and the detection of energetically efficient spacecraft trajectories.

Approximate implicitization

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Methods for finding the exact algebraic representation of rational parametric curves and surfaces are denoted implicitization. A number of well establish methods for exact implicitization exists such at resultant based methods and Groebner based method.

Floating point arithmetic is used in most industrial computer software. Exact implicitization methods implemented in floating point arithmetic gives approximate implicit curves and surfaces. In the region of computational interest the exact representation can have singular or near singular point that complicate the use of the algebraic representation. Often the use of the implicit representation is simplified if singular or near singular points are well separated from the region of computational interest. In other applications such as test for selfintersections it is important to have accurate reproduction of singularities.

Let l and g be integers with $1 \leq g < l$, and let $\mathbf{p}(\mathbf{s})$, $\mathbf{s} \in \Omega \subset \mathbb{R}^g$ be a manifold of dimension g in $\mathbb{R}^l$. The nontrivial algebraic hypersurface $q(\mathbf{x}) = 0$, $q \in P_m(\mathbb{R}^l)$, is an approximate implicitization of $\mathbf{p}(\mathbf{s})$ within the tolerance $\epsilon \geq 0$ if we can find a continuous function $\|\mathbf{g}(\mathbf{s})\|_2 = 1$ describing the direction for error measurement and a error function $|\eta(\mathbf{s})| \leq \epsilon$ such that $q(\mathbf{p}(\mathbf{s}) + \eta(\mathbf{s})\mathbf{g}(\mathbf{s})) = 0, \quad \mathbf{s} \in \Omega$.

The approximate implicitization approach is based on expressing the combination $q(\mathbf{p}(\mathbf{s}))$ as a matrix vector product $q(\mathbf{p}(\mathbf{s})) = (\mathbf{Db})^T \alpha(\mathbf{s})$. Here $\mathbf{D}$ is a matrix, $\mathbf{b}$ contains the coefficients of q and $\alpha(\mathbf{s})$ contains the basis functions related to the coordinate functions of $\mathbf{p}(\mathbf{s})$. This means that if $\mathbf{b}$ is in the null space of $\mathbf{D}$, then $q(\mathbf{p}(\mathbf{s})) = 0$. By assuming that the basis is a partition of unity we have $\|\alpha(\mathbf{s})\|_2 \leq 1$ and thus $|q(\mathbf{p}(\mathbf{s}))| \leq \|\mathbf{Db}\|_2$. The matrix $\mathbf{D}$ has desirable numeric properties if the coefficients of $\mathbf{p}(\mathbf{s})$ are contained in a simplex S, and this simplex is used for the description of q

in barycentric coordinates. When $\sigma_1 \geq 0$ is the smallest singular value of $\mathbf{D}$ we show that

$$\min_{\|\mathbf{b}\|_2=1} \max_{\mathbf{s}\in\Omega} \mid q(\mathbf{p}(\mathbf{s})) \mid \leq \sigma_1.$$

Singular value decomposition of $\mathbf{D}$ can thus be used for finding small singular values and thus an algebraic approximation of a parametric represented manifold. Constraints can be added to the algebraic approximation to control the behavior. The convergence rate of the approximation is higher than what is normal in approximation theory. Successful use of approximate algebraic surfaces depends a proper control of the gradient. Our first use of approximate implicitization was to separate near intersecting curves and surface. In the European project GAIA, IST-1999.29010, (www.math.sintef.no/gaia) we look into the potential of using approximate implicitization for detecting selfintersection. Examples of both these uses will be given.

Linear Two-point Boundary-value Problem with Polynomial Coefficients

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We consider a defect control algorithm for computing an approximate solution to a linear, second-order, ordinary differential equation with polynomial coefficients. As the boundary conditions are given at two points, we have a two-point boundary-value problem. We express the second derivative as a translated Legendre polynomial with unknown coefficients and integrate twice to find an approximate solution. We substitute the polynomial into the differential equation to compute the defect and express this defect in an orthogonal polynomial basis, using translated Legendre polynomials. Then we equate the low-order terms to zero to generate a banded system of linear equations that we solve for the unknown coefficients. In some cases we are able to approximate the solution over the entire interval with a relative error less than 10^{-100}.

Applications of SAGBI-bases to equivariant dynamics

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SAGBI bases are a tool for computing efficiently with subalgebras such as invariant rings of group actions. We generalize this concept for modules over subalgebras such as the module of equivariants. Our motivation is the usage of SAGBI bases for the organisation of algorithms in equivariant dynamics such as numerical Liapunov-Schmidt reduction and reduction onto center manifold which exploit symmetry. In both algorithms some coefficients of the equivariant polynomial vector field are computed while others are given linear equations due to symmetry. A good choice for the first set of coefficients are the coefficients of the leading monomial algebra or module, respectively. The leading monomials are given by the SAGBI basis and the linear equation are easily determined from the SAGBI basis, too.

Numerical Treatment of Overdetermined Linear PDEs

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In the first part of this talk, we show how index concepts and the notion of an underlying equation for systems of differential algebraic equations (DAEs) can be generalised to systems of overdetermined linear first order partial differential equations using the language of formal theory for PDEs. The central idea is to complete to involution the systems under consideration; if this is carried out with the perturbed system, one obtains an estimation of the perturbation index in terms of determinacy and involution indices which can be seen as refinements of differentiation indices. For involutive systems of PDEs in so-called Cartan normal form, the equations of highest class constitute the underlying equation, whereas the equations of lower class can be considered the constraints.

In the second part, we apply these methods to a certain class of linear systems called weakly overdetermined systems and examine their behaviour under semi-discretisations. Like for DAEs, the drift off the constaints can be measured for such systems. For both finite differences and spectral methods we can show that the resulting DAE is formally integrable if and only if the original system has been in involution. This inhibits the existence of hidden constraints. Finally, for general sytems we relate the index of the discretised system to certain values appearing in the completion process. This result holds also for general linear systems.

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Dynamical Aspects of Involutive Bases Computations

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In this talk we give a short introduction to involutive divisions and involutive bases computations. Different approaches are discussed and compared and a new class of involutive divisions is presented. We show results of our computer experiments with the different approaches.

Differential Equations from an Algebraic Standpoint

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Differential algebra was introduced by J.F. Ritt in the 30s as an extension of commutative algebra to differential equations. The basis theorem and the Nullstellensatz find their generalisation in this context.

Recent development have lead to effective algorithms to compute good representations of radical differential ideals generated by a finite family of differential polynomials. This representation is given as an intersection of differential ideals well defined by their characteristic sets. This representation allows to test membership to the radical differential ideal.

In other words, for a given system of ordinary or partial differential equations, the algorithms will first decide if there exist solutions. If there are, the algorithm will output a finite set of differential systems with a triangular form such that the set of solutions of the original system is equal to the union of the non singular solution set of the output systems.

With this representation, we can answer typical differential elimination questions, for instance:

- do the solutions of a system satisfy an ordinary differential equation?
- what are the differential equation satisfied by a subset of the unknown functions?
- what are the algebraic constraints?

We shall illustrate how these question arise in diverse topics.

I will also show how differential algebra contributes to the study of singular solutions of a single differential equation. For instance, for first order differential equations, we can read on the algebraic structure of the equation whether a singular solution is an envelope or a limit case of the nonsingular solutions.

A generation of the quasi-solitons in the lasers: computer algebra approach

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The modern laser technique allows the generation of sub-10 fs pulses, that is close to the fundamental limit for optical region defined by the wave period (about of 2 fs). The analysis of the lasing dynamics and properties of such pulses is a very cumbersome task, which involves a consideration of the many nonlinear factors and needs the high-performance computers for numerical simulation. Moreover, the interpretation of the obtained results is very difficult and doesn't give a clear picture of the physical processes governing laser dynamics. Therefore there is a stable interest to the analytical and semi-analytical approaches, which is induced also by the development of the efficient and universal computer algebra systems such as Maple and Mathematica. Here we present the analysis of the ultrashort pulse dynamics in the passive or active mode-locked lasers, which is based on the analytical approach and is realized as the Maple 6 package [1].

The first stage of the analysis consists in the search of the soliton-like states of nonlinear dynamical equation describing ultrashort pulse propagation. In the noncoherent case, it is, as rule, a generalized 1+1 - dimensional Landau-Ginzburg equation, which can be analyzed by Hirota's method. The presence of coherent effects due to interaction of pulse with semiconductor saturable absorber can be taking into account by two-level scheme for absorber, that results in the nonlinear dynamical equation of oscillating type, which can not be integrated by standard methods. But, as it was found, there is the approximate solution, which is close to *sech*-shaped pulse. The characteristics of the obtained solutions are in the excellent agreement with experimental observations [2]. The further analysis is based on the aberrationless approximation, which assumes the change of the quasi-soliton parameters for pulse with approximately unchanged shape. As result, we obtain the system of first-order ODE, which describes the ultrashort pulse

evolution and can be easily integrated in framework of computer algebra approach. The utilization of this approach in the analysis of the Kerr-lens mode-locked continuous-wave solid-state lasers allows to describe the experimentally observed breezers-like states with complicated dynamics (regular and chaotic) [3]. The main advantages of our approach are the possibility of the clear physical interpretation and the absence of bulk numerical computations (full computation session for different laser systems takes about of 30 min on PIII-500). Moreover the basic computational blocks can be realized as on-line Java-calculators.

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Numerical computation of Gröbner bases

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We present an installation of Buchberger's algorithm for the numerical computation of reduced Gröbner bases of a multivariate polynomial system. We are mainly interested in the case of zero-dimensional systems although the implemented algorithm can be applied in a general situation. If the system is zero-dimensional then the result of the Gröbner basis computation is used to form a multiplication matrix of the quotient ring and to solve the system numerically according to [2]. Our work is based on the installation F_4 of Buchberger's algorithm developed by J. C. Faugere [1]. We have kept the numerically attractive features of F_4 (extensive use of linear algebra and the collection of all operations with coefficients into row echelon reductions of the elimination matrix [1]); but we have improved the numerical stability of Gröbner basis computation by developing extensive selection strategies for critical pairs and reduction, and a technique for the delayed treatment of certain relations. We use a pool of superfluous relations appearing in the flow of the algorithm which are not inserted to the Gröbner basis but used by the reduction strategy routine to prevent the growth of the total degrees and of the spread in the magnitude of the coefficients in the intermediate polynomials. All selection strategies are heuristic and based on $1-$step-in-depth analysis of available choices.

Our implementation is written in C++ using idioms for emulation of symbolic language styles. It supports hardware floating point (single and double precision) as well as extra-long software emulated floating point as a domain for coefficients.

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Symbolic Techniques in Algebraic Multigrid Methods

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Part 1. The talk starts with a brief introduction to geometrical and algebraic multigrid methods (MGM) for solving large scale finite element equations approximating elliptic boundary value problems. In contrast to the geometrical MGM that is based on a hierarchy of finer and finer meshes, the algebraic multigrid (AMG) method needs only single (fine) grid information, usually the matrix and the right-hand side of the system that is to be solved. In the AMG, the hierarchy of coarser and coarser representation of the fine grid problem must be generated algebraically. There are very efficient coarsening techniques for systems where system matrix is an M-matrix.
In the paractically important case where the original system matrix is not an M-matrix, we construct an auxiliary fine grid matrix that is an M-matrix and contains all characteristical features of the original matrix. Then the coarsening is controlled by this auxiliary M-matrix. One technique of constructing this auxiliary M-matrix makes use of the element stiffness matrices of the original finite element stiffness matrix. Solving an constraint optimization problem for each finite element stiffness matrix, we find that element M-matrix that is as close as possible to the finite element stiffness matrix in the spectral sense.
Part 2. In general, we have to solve as many small constraint optimization problems as we have finite elements in our discretization. The numerical solution of all these optimization problems can be very expensive. In order to speed up the solution of these sub-problems, we solve the optimizations symbolically once and for all, and then instantiate the solutions by the local data coming from the finite elements. This accelarates the AMG solution process considerably.
In the 2-dimensional case (linear triangular elements), the symbolic solution can be computed without difficulties. The 3-dimensional case (linear tetrahedral elements) is harder because the number of variables is too large

in order to apply the available methods (Gröbner bases, resultants). However, one can get rid of several variables by re-formulating the problem in a different way, and this re-formulated problem has a short symbolic solution.

Resultants and Neighborhoods of a Polynomial

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In Computer Algebra and Symbolic Computation we deal with exact data, but in many real life situations data come either from physical measurements or observations or they are the output of numerical computations. Moreover computer works with Floating Point, i.e. with finite arithmetic, so a real number is represented approximately because of the limited number of available digits. For these reasons it is growing up the necessity of combining methods in computer algebra and numerical analysis. This led to a new branch of classic polynomial algebra, the *numerical polynomial algebra*, whose aim is to accommodate the presence of inaccurate data and inexact computation. Since a polynomial is not exact, a family of polynomials called *neighborhood* is considered as in the papers of Kaltofen and Stetter. We focus our attention on the univariate case. Let $p(x)=\sum_{j=0}^{n} a_j x^j \in \mathbb{R}[x]$ be a polynomial, the *tolerance* e associated with $p(x)$ is a non negative vector $e=\{e_0,\ldots,e_n\}$, such that $e_j \in \mathbb{R}$ and $e_j \geq 0$ for $j=0,\ldots,n$. The neighborhood $\mathcal{N}(p,e)$ of a polynomial p with tolerance e is the family of polynomials $\tilde{p} \in \mathbb{R}[x]$, $\tilde{p}=\sum_{j=0}^{n} \tilde{a}_j x^j$ such that $|\tilde{a}_j - a_j| \leq e_j$; $e_j=0$ means a_j is exact.
In this paper we give a new approach based on the idea of Resultant in order to discover the common factors between a polynomial and the polynomials in its neighborhood. Sometimes beside the acceptable variations for the coefficients of the uncertain polynomial $p(x)$, we know (often experimentally) more properties of the exact polynomial $\tilde{p}(x)$. For instance, we can know a zero of the exact polynomial, that we are looking for. So we construct $p(x)$, such that it has the same zero but it differs from the exact $\tilde{p}(x)$ in some coefficients.

Definition 1 *Let $p(x) \in \mathbb{R}[x]$ be a polynomial and let e be a vector of tolerance. The polynomial $\tilde{p}(x)$ is a* k common-factor perturbed *if $\tilde{p}(x) \in \mathcal{N}(p,e)$ and it has a common factor of degree at least k with $p(x)$. A* k

common-factor neighborhood $\mathcal{N}_k(p, e)$ *of a polynomial* $p(x)$ *is the set of all* k *common-factor perturbed.*

$Res(p, \tilde{p})$ is a homogeneous polynomial of degree $2n$ in the δ_j's and a_j's and a homogeneous polynomial of degree n as polynomial in the only δ_j's, hence by using definition as above we have the algebraic conditions on the perturbed polynomial $\tilde{p}(x)$.
Moreover given a polynomial, the Square Free property of the polynomials in its neighborhood is investigated. By using the resultant we can find the square free conditions on a polynomial $\tilde{p}(x)$ in the neighborhood.
It is also useful to see all the conditions discussed above by a geometric point of view, where the neighborhood represents a polytope and the found algebraic conditions represent hyperplanes and hypersurfaces in the space of the δ_j's (or $\tilde{a}_j$'s).

Simulation of the Three-Dimensional Blood Flow in Stenosed Coronary Arteries: Semi-Automatic Generation of the Mesh

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In current clinical practice, physicians make extensive use of medical images for diagnosing and planning therapy, but they frequently confine themselves to a visual inspection of the morphology.

The diagnosis of cardiovascular diseases and the planning of therapy should be based on a fair knowledge of the patient's hemodynamic state. This is particularly true of coronary artery disease in cases where severe stenoses in the coronary arteries increase resistance to flow. Stenoses may reduce the flow of blood to such an extent that the myocardium becomes vulnerable to ischemia. The disturbed flow around stenoses accelerates the progression of the atherosclerotic changes and may cause the formation and development of thrombi. Thus, patient-specific simulation studies of the blood flow are required which must be based on the patient's medical images (biplane angiograms).

We aim at the development of a simulation system which would allow physicians to assess their patient's hemodynamic states. This paper focuses on the semi-automatic generation of a mesh that is required for the three-dimensional simulation of the blood flow through the coronary arteries with pathological changes (stenoses) based on biplane angiograms. The simulation studies are then carried then by employing a commercial CFD software system (FIDAP).

The generated mesh fully considers the patient-specific geometry. Generating the mesh involves the acquisition of the geometry (three-dimensional reconstruction based on biplane angiograms), the creation of a meshable geometric model, and the implementation of the mesh. We aim at the generation of an optimal mesh that would allow us to compute the solution with

a specified accuracy at minimal cost in terms of computing time. To do this, we must adapt the size of the elements to the flow conditions. As a consequent adaptive procedure with an a posteriori error analysis would consume too much time, we decided to employ a priori criteria for the adaptation. Although these criteria are in principle heuristic in nature, they nevertheless reflect a fair quantitative a priori knowledge relevant to the coronary artery under investigation. This quantitative knowledge is derived from a posteriori analyses of computed flow conditions in so-called reference flow domains.

In this paper, we will give an overview of the acquisition of the geometry of the flow domain, describe our mesh generation approach, and present simulation results.

A Category Goes to Market

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Already many years ago, H.Geiger started to develop an artificial neural network (ANN) paradigm which is of great neurophysiological relevance. Intensive scientific work formed the basis of complex ANN simulations with computers that were and still are applied to hard industrial problem fields. Besides the aspects of learning it is of central interest to study the structure of the Geiger networks. This is the subject of our contribution which focuses on the mathematical (symbolic) aspects. A fruitful cooperation revealed the fact that methods from noncommutative geometry and category theory can be applied to establish a mathematical model of network structuring in a natural way. The model can be exploited to simplify ANN computer simulations in a considerable way leading to an economic effect. This could be observed and demonstrated in an industrial project on optical quality control - a reduction of production costs could be achieved by the application of the model. The overall problem solving in that project integrated symbolic and numerical methods. We briefly describe this project at the end of our contribution. In this sense a "category went to market".

A Symbolic-Numeric Algorithm for Computing Approximate Solutions of First-order Formulae over the Reals.

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Traditionally, first-order formulae over the reals have been solved by purely symbolic methods, such as quantifier elimination by cylindrical algebraic decomposition. In the talk we will introduce a mixed symbolic-numeric algorithm that avoids the costly algebraic number computation of purely symbolic approaches. The algorithm assumes that each variable ranges over a predefined interval. It follows a branch and prune scheme in which branching splits the range of a variable into pieces, and pruning extracts useful information from the input formula while reducing the range of its variables. By relying on validated arithmetic the algorithm can still provide provably correct results, and terminates for those inputs that are numerically well-posed.

Symbolic Methods for the Equivalence Problem of Systems of Implicit Ordinary Differential Equations

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This contribution deals with the equivalence problems for systems of implicit ordinary differential equations of the following type

$$f^{i_e}\left(t, z, \dot{z}\right) = 0 \ , \quad i_e = 1, \ldots, n_e \tag{1}$$

with $z \in \mathbb{R}^q$, $q \leq n_e$. The time derivative of z is denoted by $\dot{z}$. Equivalence means that every solution of the original set of equations is a solution of some normal form and vice versa

$$\dot{x}^{i_e} = f^{i_e}\left(t, x, u\right) \ , \qquad \dot{x}^{i_e} = f^{i_e}\left(t, x, u^{(n)}\right) \ ,$$

where the variables x describe the *state* and u the *input* of the system. The symbol $u^{(n)}$ indicates that derivatives up to the order n of the input are admissible. The mathematical investigations are based on the theory of jet-bundles [1], the system (1) is identified with the submanifold in a suitable jet-space, defined by the equations. This approach allows us to combine methods from differential geometry and elimination theory.

The equivalence problem will be solved for the well-determined case, where the number of equations n_e and unknowns q is equal, as well as for the under-determined case with $q - n_e = 1$. For the case $q - n_e > 1$ several solutions will be presented, but we leave the problem open, how to minimize the number of inputs, whose derivatives appear in the normal form. Apart from the theoretical results we present several sketches for computer algebra based algorithms that are necessary to solve these problems efficiently.

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Symbolic Summation in Difference Fields

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There are implementations of the celebrated Gosper algorithm (1978) on almost any computer algebra platform. Within my PhD thesis work I implemented Karr's Summation Algorithm (1981) based on difference field theory in the Mathematica system. Karr's algorithm is, in a sense, the summation counterpart of Risch's algorithm for indefinite integration. Besides providing a new approach to Karr's algorithm which allows us to find closed forms for a big class of multisums, I developed new extensions to handle also definite summation problems. More precisely I am able to apply creative telescoping in a very general difference field setting and are capable of solving linear recurrences in its context. In particular, I designed algorithms for finding appropriate difference field extensions to solve problems in symbolic summation. For instance I deal with the problem to find all nested sum extensions which provide us with additional solutions for a given linear recurrence of any order. Furthermore I find appropriate sum extensions, if they exist, to simplify nested sums to simpler nested sum expressions.

Algorithmic Lie Theory for Solving Ordinary Differential Equations

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In the second half of the 19^{th} century Sophus Lie developed a theory for solving differential equations in analogy to Galois's theory of solving algebraic equations in terms of radicals. As an auxiliary device he established his theory of continuous groups, known as Lie-groups today, and its corresponding Lie-algebras.

In principle Lie's theory applies to differential equations of arbitrary order. However if the goal is to design solution algorithms based on this theory that may be implemented in a computer algebra system, several steps have to be worked out in more detail. To this end it is supplemented by two basic concepts:

1. Janet bases for systems of linear partial differential equations that determine the symmetry generators of a given differential equation and the transformation to canonical forms.

2. The decomposition of these Janet bases into irreducible components by Loewy's theory in analogy to the decomposition of ordinary linear differential equations.

Proceeding in this way completely algorithmic procedures are obtained for obtaining closed form solutions of equations with symmetries the solutions of which are contained in well-defined function fields. The basic steps involved are reviewed. Complete results are presented for second- and third order ordinary differential equations. Various possible extension are discussed, e.g. equations of order four or higher, and certain types of partial differential equations.

Software Demo: On top of the algebraic type system ALLTYPES, software for working with differential equations has been developed with special emphasis on Lie's symmetry theory. It is shown how the use of this software makes available many of these concepts that could not be used by conventional pencil-and-paper methods.

NONLINEAR WAVES IN SHALLOW WATER

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The scaled surface wave equations for horizontal and vertical velocities $u(x,z,t)$ and $w(x,z,t)$ read:

$$\mu^2 u_x + w_z = 0 \quad , \quad -sx < z < \varepsilon\eta(x,t) \tag{1}$$

$$\eta_t + \varepsilon u\eta_x - \mu^{-2} w = 0 \quad , \quad z = \varepsilon\eta(x,t) \quad , \tag{2}$$

$$u_t + \varepsilon\left(uu_x + \mu^{-2} ww_x\right) + \eta_x = 0 \quad , \quad z = \varepsilon\eta(x,t) \quad , \tag{3}$$

$$w = -\mu^2 h_x u \quad , \quad z = -sx. \tag{4}$$

where $\varepsilon = a_0'/h_0'$, $\mu = h_0'/l_0'$ and a_0', h_0', l_0' are a characteristic wave amplitude, water depth, and wavelength, respectively. For the depth-averaged velocity $U \equiv \left(\int_{-h}^{\varepsilon\eta} u dz\right) / (h + \varepsilon\eta)$, Boussinesq-type equations retaining terms of orders $O(\mu^2)$ and $O(\varepsilon)$ were derived by Peregrin (1967). The work by Madsen & Schäffer (1998) contains an algorithm for constructing a series of the Boussinesq-type equations $\mathcal{B}_m$ retaining ε^m, $\varepsilon^{m-1}\mu^2$, ... , μ^{2m} terms. We consider the equations $\mathcal{B}_2$ for the case of sloping bottom in some area, excluding the deep water region where the shallow water restrictions are violated.

$$\mathcal{B}_2 : U_t + \eta_x + \varepsilon UU_x + \mu^2\left(-s^2 xU_{xt} - \frac{1}{3}s^2x^2U_{xxt}\right) +$$
$$\varepsilon\mu^2\left(-sU_t\eta_x - sU_{xt}\eta - sxU_{xt}\eta_x - s^2xUU_{xx} + \frac{1}{3}s^2x^2U_{xx}U_x - \frac{2}{3}sx\eta U_{xxt} - \frac{1}{3}s^2x^2U_{xxx}U\right) +$$
$$\mu^4\left(-\frac{4}{9}s^4x^2U_{xxt} - \frac{2}{9}s^4x^3U_{xxxt} - \frac{1}{45}s^4x^4U_{xxxxt}\right) = 0 \tag{5}$$

$$\eta_t + ((h + \varepsilon\eta)U)_x = 0 \tag{6}$$

The depth-averaged velocity U and surface elevation η are periodic and expanded in Fourier series with frequency ω. The major finding is the explicit expressions, found by computer, for the coefficients of the first four harmonics of the Fourier series calculated up to the orders ε^3, $\varepsilon\mu^2$, and μ^4 inclusively. They are polynomials of Bessel functions $J_0\left(2\omega\sqrt{\frac{x}{s}}\right)$, $Y_0\left(2\omega\sqrt{\frac{x}{s}}\right)$, $J_1\left(2\omega\sqrt{\frac{x}{s}}\right)$, $Y_1\left(2\omega\sqrt{\frac{x}{s}}\right)$ whose coefficients are polynomials of $x^{\frac{1}{2}}$ and $x^{-\frac{1}{2}}$. This result is closely related to note [3], where case of standing waves is considered

We conjecture that periodic solutions to $\mathcal{B}_m$ over a slope can be found as expansions of the form:

$$C^0(x) + S^1(x)\sin(\omega t) + C^1(x)\cos(\omega t) + ... + S^m(x)\sin(m\omega t) + C^m(x)\cos(m\omega t) + ... \tag{7}$$

where $S^m(x)$ and $C^m(x)$ are polynomials of Bessel functions $J_0\left(2\omega\sqrt{\frac{x}{s}}\right)$, $Y_0\left(2\omega\sqrt{\frac{x}{s}}\right)$, $J_1\left(2\omega\sqrt{\frac{x}{s}}\right)$, $Y_1\left(2\omega\sqrt{\frac{x}{s}}\right)$ whose coefficients are polynomials of $x^{\frac{1}{2}}$ and $x^{-\frac{1}{2}}$.

Velocities $u(x,z,t)$ and $w(x,z,t)$ can be expressed in terms of U, η, and their derivatives which permits to interpret the result as a periodic solution to classical wave problem (1) - (4) over a slope found up to the orders ε^2, $\varepsilon\mu^2$, and μ^4. This allows to conjecture that exact periodic solutions to the problem (1) - (4) can be described as a power series in z with coefficients of the form (7).

Numerous numeric results illustrating the presented method are included

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Algebraic Predicates for Empirical Data

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It is widely assumed that the assignment of truth values to non-trivial algebraic predicates containing numerical data is possible only if the data are exact and if exact computation is employed. But in many *application areas* the answers to questions like "Are all zeros of that (model) polynomial in the left half-plane?" are of principal importance.

We develop a framework in which algebraic predicates with *empirical data* are assigned a positive real number in place of a truth value. This *validity value* permits an interpretation which is more informative that the classical "yes – no" answer. It depends *continuously* on the data and can thus be computed approximately by floating-point arithmetic. A number of non-trivial examples support the usefulness of our approach.

Solving Symbolic and Numerical Problems in the Theory of Shells with *MATHEMATICA*®

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The aim of the lecture is to show how, thanks to the computer algebra system *MATHEMATICA*® [1] and its external package ***MathTensor***™ [2], it is possible to solve symbolic and numerical tasks in the theory of shells.

The lecture will cover the following problems:

1. **Computer assisted tensor analysis of shell tasks**
   Application of the computer algebra system to solve tensor symbolic problems. Derivation of *MATHEMATICA*® differential equations from tensor ones. Receiving and simplification of the constitutive relations and strain energy density. Numerical examples.

2. **Shell geometry with *MathTensor*™**
   Application of ***MathTensor***™ to translate relations of differential geometry to the *MATHEMATICA*® language.

3. **Description of an arbitrary shell**
   Geometrical properties, kinematic relations, strains, internal forces and differential equations.

4. **Shells boundary value problems with least squares method**
   The refined least squares method was implemented into the computer algebra. The method is very useful for the boundary value problems of shells as they are typical problems of boundary layer. The advantages of the method.

[1] *MATHEMATICA*® is a product of Wolfram Research, Inc.
[2] ***MathTensor***™ is a product of MathSolutions, Inc.