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ABSTRACTS

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Contents

Preface

This volume contains peer refereed abstracts of the 13th GAMM-IMACS International Symposium on Scientific Computing, Computer Arithmetic and Verified Numerical Computations, El Paso, Texas, September 29 – October 3, 2008. The goal of SCAN 2008 is to advance the frontiers in verified numerical computations, as well as in their application to computational engineering and science. Topics of interest include, but are not limited to:

- Hardware and software support for verification tools
- Theory, algorithms and arithmetic for verified numerical computations
- Supercomputing and reliability
- Dynamical systems and verified numerical computation
- Global optimization and verified numerical computation
- Programming tools for verified numerical computation
- Computer aided proofs
- Industrial and scientific applications of verified numerical computations

The conference continues the series of international SCAN symposia held under the joint sponsorship of

- GAMM (International Association of Applied Mathematics and Mechanics) and
- IMACS (International Association for Mathematics and Computers in Simulation).

These symposia have covered the numerical and algorithmic aspects of scientific computing, with a strong emphasis on verification of computed results, as well as on arithmetic, programming, and algorithmic tools for this purpose. Their objectives have been both to propagate current applications and research and to promote a greater understanding and increased awareness of the subject matters. These symposia have been initiated by the University of Karlsruhe, Germany. They have been held in many cities across the world:

- Basel, Switzerland (1989)
- Albena, Bulgaria (1990)
- Oldenburg, Germany (1991)
- Vienna, Austria (1993)
- Wuppertal, Germany (1995)
- Lyon, France (1997)
- Budapest, Hungary (1998)
- Karlsruhe, Germany (2000)
- Paris, France (2002)
- Fukuoka, Japan (2004)
- Duisburg, Germany (2006)

SCAN 2008 intends to be a forum for the researchers of various fields in numerical verification to discuss many existing verification tools and approaches.

We want to use this opportunity to thank all the contributors and participants of this workshop. This volume contains papers authored by researchers from all over the world, from Belgium, Brazil, Bulgaria, Canada, P.R. China, Chile, Czech Republic, France, Germany, Hungary, India, Japan, Russia, Serbia, South Africa, Spain, Taiwan, Ukraine, UK, and the USA. Without their active participation, we would not have succeeded.

We also want to thank researchers from the Cyber-Share Center (supported by NSF Grant HRD-0734825) for their help.

Martine Ceberio, Vladik Kreinovich, and Scott A. Starks
Local Organizers

Machine-Efficient Chebyshev Approximation for Standard Statistical Distribution Functions

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When implementing a real function such as sin, cos, etc. on any computing system, polynomial approximations are almost always used to replace the actual function. The reason behind this is that addition, subtraction, and multiplication are efficiently implemented in general-purpose processors [2].

In this paper we extend the idea of Brisebarre, Muller, Tisserand, and Chevillard on machine-efficient Chebyshev approximation [2,3]. Our extensions include standard statistical distribution functions, by which we mean: the normal distribution, the beta distribution, the F-distribution, and the Student's t-distribution. We choose Chebyshev polynomials as they provide a good polynomial approximation [1,5]. These practical calculations have been performed using Müller's iRRAM [6].

The standard statistical distribution functions are important functions that are used in probability theory and statistics [4]. Finding an efficient way of approximating these functions would be beneficial. The (cumulative) normal distribution function N(0,1) with mean 0 is defined by the following Equation

$$N_{0,1}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{1}{2}u^2}\, du \tag{1}$$

On the other hand, the beta distribution function is defined in Equation (2). It is defined in the interval [0,1] with two positive shape values α and β.

$$F(x;\alpha,\beta) = \frac{B_x(\alpha,\beta)}{B(\alpha,\beta)} = I_x(\alpha,\beta) \tag{2}$$

where $B_x(\alpha,\beta)$ is the incomplete beta function, $B(\alpha,\beta)$ is the beta function, and $I_x(\alpha,\beta)$ is the normalized incomplete beta function [4].

The F-distribution function is defined in Equation (3). It is defined in the interval [0,∞] with the degree of freedom values v_1 and v_2.

$$Q(F|v_1,v_2) = I_x\left(\frac{v_1}{2},\frac{v_2}{2}\right) \text{ , where } x = \frac{v_1 F}{v_1 F + v_2} \text{ and } F \geq 0, v_i > 0. \tag{3}$$

The Student's t-distribution is a special case of the F-distribution and is defined in Equation (4):

$$A(t|v) = 1 - I_x\left(\frac{v}{2},\frac{1}{2}\right) \text{ , where } x = \frac{v}{v+t^2} \text{ and } v > 0. \tag{4}$$

The first step of getting the machine-efficient Chebyshev approximation is to calculate the Chebyshev series that approximate the required functions. The next step is to convert the standard approximation into a machine-efficient version. We implement the machine-efficient Chebyshev approximation as shown in Equation (5):

$$f(x) \approx \sum_{n=0}^{\infty} \frac{a_n}{2^m} x^n \text{ where } a_0, ..., a_n \in \mathbb{Z}, \text{ and } m \in \mathbb{N}. \tag{5}$$

The machine-efficient Chebyshev approximation can approximate the above functions with a defined error. We found that these machine efficient approximations do indeed improve the efficiency with which these operations can be performed. The total error (E_t) of performing the machine-efficient approximation is defined in Equation (6):

$$E_t = \text{machine-efficient error} + \text{approximation error}. \tag{6}$$

The machine-efficient error that is caused by converting the standard Chebyshev approximation to machine-efficient Chebyshev approximation. This error is defined in Equation (7):

$$\text{Machine-Efficient error } = n \cdot \frac{1}{2^m}, \tag{7}$$

where n is the order of Chebyshev approximation, and $m \in \mathbb{N}$ that represents the accuracy of the coefficients.

The approximation error is defined in Equation (8):

$$|f(x) - P_n(x)| \leq \frac{2(b-a)^{n+1}}{4^{n+1}(n+1)!} \max_{a \leq x \leq b} |f^{n+1}(x)|, \tag{8}$$

where a, and b are the end points of the interval [a,b], and n is the order of interpolating polynomial $P_n(x)$ [1].

Instead of doing forward error analysis, Equation (6) can be used to perform this type of approximation in an exact arithmetic framework.

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Keywords: Approximation Theory, Chebyshev Polynomial, Computable Functions, Computable Real Arithmetic, Machine-Efficient Polynomial, Numerical Analysis.

On the Interval Cholesky Method

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Enclosing the set S of solutions of linear systems $Ax = b$ is one of the main topics in interval analysis. Here A is an $n \times n$ matrix and b is a vector with n components which both are allowed to vary within given interval bounds. In many applications the matrix A is restricted to a symmetric matrix which leads to the so–called symmetric solution set $S_{\rm sym}$. Since usually $S_{\rm sym}$ is a proper subset of S one tries to find interval enclosures for $S_{\rm sym}$ which need not be enclosures for S at the same time. Among others the interval Cholesky method provides an enclosure $[x]^C$ which can be such a better enclosure of $S_{\rm sym}$.

For symmetric positive definite point matrices A it is well known that the Gaussian algorithm (without pivoting) is applicable if and only if the Cholesky method is applicable. In our talk we study a similar relation between the corresponding interval version of both algorithms. Moreover, we extend the catalogue of criteria for the applicability of the interval Cholesky method. It turns out that the interval Cholesky method is applicable whenever the interval Gaussian algorithm is, provided that $[A] = [A]^T$ contains a symmetric and positive definite element matrix. Unfortunately, the converse is only true for dimensions $n \leq 3$. That it fails for $n > 3$ is shown by an example. This astonishes somewhat since the Gaussian algorithm is applicable for all point matrices in $[A]$ if $[x]^C$ exists and n is arbitrary. For particular classes of matrices the applicability of both algorithms is equivalent for any dimension. Among them are the generalized diagonally dominant matrices, tridiagonal matrices, and matrices of the form $[A] = I + [-R, R]$ which one gets when preconditioning interval matrix and righthand side by the midpoint inverse of $[A]$. For generalized diagonally dominant matrices we list alternative criteria for the applicability which involve the signs of the midpoint matrix of $[A]$ – eventually modified in a prescribed way.

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Bounding the Error for Approximate Solutions of Almost Linear Complementarity Problems Using Feasible Vectors

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In this paper we use the concept of a feasible vector in order to prove the existence of a solution x^* of an almost linear complementarity problem in a certain set. This proof delivers also componentwise error bounds for an approximation $\hat{x}$ to a solution x^*. In the special case that the problem is defined by a so-called H-matrix, we prove that the error bounds are more accurate than certain corresponding bounds recently obtained. By numerical examples it will be demonstrated that the new bounds can be better by several orders of magnitude.

Keywords: Complementarity problem, H-matrix, error bound

Mathematics Subject Classification (2000): 90C33, 65G30, 65K10

On the Accuracy of the CELL Processor

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The CELL parallel processor has been jointly designed by IBM, Sony and Toshiba for the playstation 3. Thus it has mainly been designed for high speed rather than accurate computing, as the purpose was a very fast processing of images. Anyhow it is also used to build super computers as the IBM Roadrunner which is made up of a blend of 12,960 modified Cell processors and some 6948 AMD Opterons and has broken the computing record in june 2008 with more than 1 petaflops. Actually the heart of a CELL is a main processor and 8 high speed parallel processors on a single chip. As speed is the main goal, the floating point arithmetic of the 8 parallel processors work with chopping (rounding to zero) arithmetic and does not posses the 4 rounding modes of the IEEE754 standard. Only the main processor has a floating point arithmetic according to this standard. The consequence of this choice is that computing with the 8 parallel processors of the CELL may be much less accurate than with a processor with a rounding to nearest arithmetic, particularly when dealing with linear algebra.

It has been shown in [1,2], that the computational complexity and thus the computation time of an inner product of n components is proportional to n when the processor has a chopping arithmetic and to $\sqrt{n}$ with a rounding to nearest arithmetic. Similarly it has been shown in [3,4] that when the data are unprecise and belong to some known gaussian distribution $N(\mu,\ \sigma)$ they can be modeled by so-called stochastic numbers and the computation on them by stochastic arithmetic which is operations on gaussian distributions. With such stochastic numbers the error on the result of the sum of n numbers is also proportional to $\sqrt{n}$. This is in fact an illustration of Wilkinson's backward error analysis in which approximate computation on exact data are viewed as exact computation on some perturbed data. Stochastic arithmetic is in fact a model for the random rounding arithmetic which is implemented in the Cestac method and the Cadna Software [5,6]. In this paper some numerical experiments are given to compare the rounding to zero arithmetic of the CELL processor, the rounding to nearest arithmetic of a processor working with the IEEE754 norm and the stochastic arithmetic of the Cestac Method. It is then shown that, in linear problems, rounding to zero provides an error proportional to $O(n)$ whereas rounding to nearest and stochastic arithmetic provide an error in $O(\sqrt{n})$. The consequence is that, as this processor is designed for solving very large problems very fast one must be careful concerning the accuracy of the results.

Keywords: Linear algebra, round-off error, CESTAC method, stochastic arithmetic.

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Using Intervals for the Concise Representation of Inverted Repeats in RNA

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Ribonucleic acid, or RNA, is a nucleic acid consisting of a long sequence of chained nucleotide units. Nucleotides consist of a sugar, a phosphate group, and a nitrogenous base, which in RNA is generally adenine (A), cytosine (C), guanine (G) or uracil (U). RNA plays many important roles within a cell, for example, messenger RNA (mRNA) carries the protein-building blueprint from the DNA template to the ribosomes (the protein-building sites); transfer RNA (tRNA) transfers aminoacids (the protein-building blocks) to the ribosomes; and ribosomal RNA (rRNA), the central component of the ribosome, decodes mRNA and builds the protein by chaining together the aminoacids transferred by tRNA.

To achieve functionality, RNA molecules often require a specific tertiary structure, defined by the three-dimensional atomic coordinates. The scaffold for the tertiary structure is provided by the secondary structure, defined by the hydrogen bonds between nitrogenous bases. In RNA, typically cytosine (C) bonds with guanine (G) and adenine (A) bonds with uracil (U), although other base-pairs are possible.

Most RNA secondary structures are defined by these base-pairings between nucleotides. If we represent an RNA molecule as a string over the alphabet [GUCA], the RNA molecule 'GUCACCCCUGAC' can base-pair positions 1-4 with positions 9-12 and create a stem-loop (where the pairs form the stem, or helix, and the unpaired positions form the loop), a common secondary-structure pattern that is a building-block for more complex secondary structures.

Several approaches to secondary structure prediction consider finding these palindromic inverted repeats, which equate to base-pairs in a molecule. For example, EMBOSS ("European Molecular Biology Open Software Suite") provides a *palindrome* utility that searches for inverted repeats.

Results from EMBOSS's palindrome utility are correct but sometimes not very concise. For example, for a sequence 'AAAACCCCUUUUUUUUU', palindrome reports possible base-pairings 1-4:9-12, 1-4:10-13, 1-4:11-14, 1-4:12-15, 1-4:13-16, 1-4:14-17, and 1-4:15-18. If we use intervals to represent this data, we can report instead base-pairs [1, 4]:[9, 18].

The approach can be extended to more complex sequences where the helices consist of more than one base. For example, for a sequence 'CAAAACCCCUUUUUUUUUUG' we have pairings [1-5]:[10-20] with bulges of sizes [0-6]. Bulges arise because stem-halves need not be continuous, for example, we can have, in the above sequence, pairings 1:20 and 2-5:14-17, with positions 18 and 19 being in a bulge. Further constraints, such as reasonable loop and bulge sizes can be developed as well, also using intervals.

Verification and Validation of Two Biomechanical Problems

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Biomechanics is an important research area in applied physics. The studies in this field range from investigating the behavior of cells to simulating the movement of (human) limbs. In particular, biomechanics supports physicians in assessing a therapy before applying it to a patient. However, it is difficult to perform exact measurements on living objects and, consequently, obtain parameters for biomechanical models which would guarantee the correctness of simulations for a specific person. That is why such problems are a challenging application area for interval methods since they help to assess the model uncertainty in a (theoretically) efficient way aside from providing verified results.

In this talk, we consider two practically relevant biomechanical problems: identification of body segment motion using marker trajectories and identification of muscle activation profiles. New double precision methods, which do not take into account uncertainties, have been developed recently for both of these tasks by A. Kecskeméthy's group (University of Duisburg-Essen) [1]. The goal of our team is to obtain enclosures for the hip joint position and femur length from the recorded but inexact data on positions of markers attached to the patient's leg for the first problem. In the second, more complex dynamical case, we not only consider *verification* of the hip and knee angle trajectories of a human leg over time under the influence of various uncertain parameters, but also try to *validate* it against the reality of (discrepant) gait lab data. The challenges here are the overestimation resulting among other reasons from the chaotic nature of the underlying model and the necessity to work with functions which are differentiable only piecewise.

We start by describing the verification and validation assessment cycle and a formal way to analyze a (bio)mechanical process from the point of view of certification and verification of its parts. After that, we present the results for the above mentioned problems. Here, we compare additionally the numerical and symbolic approaches to verification of the behavior of mechanical systems using SmartMOBILE [2] and a MoMaple-based tool, respectively. An outlook on future tasks and challenges in this field concludes this talk.

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Keywords: biomechanics, numerical verification assessment, uncertainty, result verification

Comparing Inclusion Techniques on Chemical Engineering Problems

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Solving general nonlinear systems of equations and/or finding the global optimum of nonconvex functions constitute an important part of the everyday practice in chemical engineering. Standard methods cannot provide theoretical guarantee for convergence to a solution, cannot find multiple solutions, and cannot prove non-existence of solutions. This is the main motive to apply interval methods. Interval analysis has been applied to a wide variety of problems in chemical engineering, *e.g.* [1]. Similarly impressive results can be achieved with αBB, a fairly general global optimization method [2, 3].

Computing steady states of multistage separation processes requires solving large-scale nonlinear systems of equations. Despite of the outstanding results referred above, computation of these problems with interval arithmetic have not yet been considered in the literature, according to the authors' best knowledge. The only globally convergent methods used in this area seem to be the homotopy-continuation methods [4]. Leading edge software packages, such as [5], are also available to find zeros of nonlinear systems. Unfortunately, finding all solutions can be guaranteed only in special cases *e.g.* polynomial systems with no constraints [6].

The authors aim to compute steady states of homogeneous and heterogeneous azeotropic distillation columns with interval methods, keeping the algorithm as problem independent as possible. The results achieved so far are presented here.

Numerical evidence published in the literature, *e.g.* [7, 8], seem to indicate superiority of the linear interval approximation (LIA, $\boldsymbol{L}(x) = Ax + \boldsymbol{b}$, A is a real matrix), proposed by Kolev in a number of publications *e.g.* [9], compared to the traditional interval linear approximation (ILA, $\boldsymbol{L}(\boldsymbol{x}) = \boldsymbol{A}(\boldsymbol{x} - z) + f(z)$, $\boldsymbol{A}$ is an interval matrix) such as the interval Newton method. LIA has the following advantages over ILA when applied to root-finding. (*i*) The solution set of the LIA has a much simpler form, the hull solution is straightforward: $\boldsymbol{X} \cap -A^{-1}\boldsymbol{b}$. (*ii*) Linear programming is directly applicable to prune the current box. The automatic computation of LIA is possible with affine arithmetic [10] which in turn (*iii*) automatically keeps track of correlation between the computed partial results yielding tighter enclosures. There is no significant difference in the computation time per iteration between LIA and ILA.

In [11] LIA and ILA are compared as linearization techniques applying them to chemical engineering problems of real complexity. The examples considered are highly structured and are full of dependency. LIA outperforms the traditional 'textbook' interval Newton algorithm (IN/GS) by an order of magnitude in the case of the studied examples. Note that *state-of-the-art* variants of the interval Newton methods, *e.g.* [12, 13], also outperform the IN/GS used for comparison. Linear programming may be preferable as pruning technique for LIA because of its robustness. Considering the conclusions of [11], the C++ class has been re-implemented, and the LP pruning

method has been revised. The improvement is significant; real life medium-scale problems are successfully solved. Some of the problems used for comparison are suitable for benchmarks, they will be contributed soon.

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Keywords: affine arithmetic, linear programming, root finding, branch-and-prune, dependency problem

Preserving Privacy in Statistical Databases by Using Intervals Instead of Cell Suppression

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An important challenge with statistical databases is to protect the privacy of an individual when aggregate data is released. Cell suppression is a commonly used technique to this end. This involves the suppression of additional non-sensitive data to restrict inferences about the sensitive data.

We suggest another approach which we call cell blurring. Instead of completely suppressing some cells, we can replace the value in a cell by an interval. This has the advantage of distributing the uncertainty introduced by the suppression more evenly across the entire data. We propose a number of algorithms that, given a statistical database, a table to be published, some cells in the database that are considered sensitive and a degree of privacy that needs to be guaranteed on the sensitive cells, and computes a new table of intervals that may be published while preserving privacy.

A Computer-Assisted Proof for Stable/Unstable Behaviour of Periodic Solutions for the Forced Damped Pendulum

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We consider a simple mechanical system, the forced damped pendulum. According to earlier publications [3] this system has chaotic behaviour. Among other things, the chaotic behavior is implied by the existence of an unstable periodic solution.

First we describe an automatic technique that is able to enclose periodic solutions. To find such regions that satisfy the respective conditions, we applied an interval inclusion and a recursive subdivision technique. In the considered system we find two periodic solutions. One of them is unstable and the other one is stable. The unstable 2π-periodic solution is bifurcated from the top equilibrium position, and the other, asymptotically stable 2π-periodic solution is bifurcated from the bottom equilibrium position of the damped unforced pendulum.

To find out whether the periodic solution is stable, we can calculate the Jacobian matrix for the related variables and analyze their eigenvalues. Unfortunately, the Jacobian matrix of this pendulum cannot be given in closed form. One of the possibilities is to apply the characteristic multiplicator technique. To this end we can determine the Poincaré map, and while we follow the trajectory [2], we calculate the derivatives as well. Rounding and other errors were considered, both in the trajectory following and in the calculation of eigenvalues. With this method we can provide the anticipated result for the mentioned 2π-periodic solutions [1].

Finally, we discuss some stabilization techniques. We analyze how to stabilize the unstable periodic solution of the considered pendulum. One of these methods uses the current values of the state variables (the angle and the speed of the pendulum), thus this is a feedback control. The other method does not use this kind of information, so it is not a feedback control. We also analyze whether these methods really stabilize the unstable solution. We are able to prove necessary conditions for the stabilization of the unstable solution.

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Keywords: computer-assisted proof, periodic solutions, forced damped pendulum, control

Box Satisfaction and Unsatisfaction for Solving Interval Constraint Systems

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In [1,2], we introduced two new concepts to interval constraints and interval analysis: box satisfaction and box unsatisfaction. Box satisfaction starts with a box B contained in the solution set, and enlarges B to obtain a "maximal" box in the solution set. Box unsatisfaction starts with a box D that does not contain any solutions, and enlarges D to obtain a "maximal" box containing no solution. The initial boxes B and D can be singletons. In this paper, we show how to solve interval constraint systems using these two concepts, and their relaxed versions. We also provide a `C++` implementation for that.

Two approaches are used in our implementation: top-down and bottom-up. In the top-down approach we start from the box B in which the solutions are sought. Propagation and/or box consistency algorithms are then applied to reduce B. If we succeeded in shrinking B, the parts deleted are enlarged using box unsatisfaction to further shrink the search space. The remaining domain is then split into a set of boxes and the process is repeated on each box. If a box D is contained in the solution set, box satisfaction is used to enlarge parts of D. This helps to further reduce the search space by enlarging the solution set.

The bottom-up approach uses classical numerical methods to find solutions (non-solutions) to the interval constraint system. We then enlarge their results using box satisfaction (box unsatisfaction). If a "solution" returned by a classical method cannot be proven to be a solution, or the classical method diverges, our algorithm randomly generates the next box to check. The process is repeated until the whole search space is covered. Other criteria for stopping are also investigated.

Both approaches generates two lists: the list of boxes contained in the solution set, and the list of boxes containing no solution. The set difference between the initial box and the union of the boxes in both lists is the un-decidable region.

To help visualize the two approaches, our implementation offers graphical capabilities to dynamically view them in two dimension. Two benchmarks are used to test our implementation.

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[**2**] Belaid, M.; *Box satisfaction and Unsatisfaction*, submitted to Reliable Computing Journal, 2007.

Keywords: Interval constraints, box satisfaction, box unsatisfaction, CSP.

A Unified Interval Constraint Framework for Crisp, Soft, and Parametric Constraints

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In this paper we present a unified framework for handling different kinds of interval constraint systems, namely crisp constraints, soft constraints [4,5], and parametric constraints [1,2,3]. The framework allows for applying different propagation algorithms [1], especially clustered propagation algorithms, and dual propagation algorithms. The unified framework is implemented and used to solve a flight-envelope clearance problem. The implementation uses several design patterns and is available under GNU General Public License (GPL).

In the addition to variables, a constraint may involve parameters. A parameter has an interval associated with it. As a special case, if the parameter is a constant a, then its interval is $[a_l, a_r]$, where a_l is the greatest floating-point less than or equal to a, and a_r is the smallest floating-point greater than or equal to a. Since we will be dealing with robust solutions, i.e., solutions that satisfies all the constraints for all the values of the parameters, parameters are handled as universally-quantified variables.

To each constraint C, we associate a softness level. Level 0 means that the constraint C is crisp, and Level 1 implies that C must be removed from the constraint system. Each variable has an existence level. Only levels with two values are considered in this paper. Level 0 means that the variable is a parameter, i.e., a variable with universal quantifier, and Level 1 means a variable with existential quantifier. For each constraint C and variable v, we associate a domain reduction operator (DRO), $dro(C, v)$, that depends on the expression of C, its level, the variable v, and its level.

In our implementation, the softness of a constraint C is handled using two techniques: limiting the number of times the DRO of a constraint is called, and relaxing the reductions introduced by its DRO on the domains of the variables involved in C.

The duality between the existential and the universal quantifiers leads us to a straightforward implementation of parametric constraints. In fact, for an existential variable v, if a DRO reduces the domain of v to empty, then the system of constraints does not have any solutions. For a parametric variable, this happens when its domain is reduced. In other words, after applying a DRO, if the domain of the parametric variable shrinks, then the constraint system does not have any solutions. For inequalities, our framework can prove that a whole box is a subset of the solution set. This fact is also used in the implementation of parametric constraint systems.

After presenting the theoretical foundations of our framework, we show how to implement it in *C++* using few design patterns. The implementation is used to solve a practical problem, namely a flight-envelope clearance problem. The graphical capabilities of our implementation is used to visualize the solutions of the problem.

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Keywords: Interval constraints, parametric constraints, soft constraints, crisp constraints, domain reduction operator, CSP.

Staggered Correction Computations with Enhanced Accuracy and Extremely Wide Exponent Range

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A so called staggered precision arithmetic is a special kind of a multiple precision arithmetic based on the underlying floating-point data format (IEEE double format), [1],[2],[3]. In C-XSC a staggered interval $\boldsymbol{x}$ with a precision p is defined as an array of $p+1$ components:

$$\boldsymbol{x} := \sum_{i=1}^{p-1} x_i + [x_p, x_{p+1}] = [\mathtt{Inf}(\boldsymbol{x}), \mathtt{Sup}(\boldsymbol{x})] = [\underline{\boldsymbol{x}}, \overline{\boldsymbol{x}}],$$

$$\mathtt{Inf}(\boldsymbol{x}) := \sum_{i=1}^{p-1} x_i + x_p, \quad \mathtt{Sup}(\boldsymbol{x}) := \sum_{i=1}^{p-1} x_i + x_{p+1}.$$

The basic arithmetic operations are based on the known C-XSC data type `dotprecision` (so called long accumulator) and so, e.g. the machine product $\boldsymbol{x} \diamond \boldsymbol{y} \ni \boldsymbol{x} \cdot \boldsymbol{y}$, results in an optimal enclosure of the exact interval $\boldsymbol{x} \cdot \boldsymbol{y}$. However, even with a high precision p the accuracy of $\boldsymbol{x} \diamond \boldsymbol{y}$ may be reduced drastically, if $\boldsymbol{x} \cdot \boldsymbol{y}$ lies near the underflow range. Moreover, the program is aborted, if the value of the dot product lies in the overflow range.

To avoid these disadvantages the extended staggered arithmetic uses an additional factor 2^r, $r \in \mathbb{Z}$:

$$(r, \boldsymbol{x}) := 2^r \cdot \boldsymbol{x} = 2^r \cdot \left(\sum_{i=1}^{p-1} x_i + [x_p, x_{p+1}] \right).$$

With r of type `double` an extremely wide range of the exponents r is realized:

$$-9007199254740991 \leq r \leq +9007199254740991 = 2^{53} - 1.$$

The greatest absolute value of an interval $\boldsymbol{x}$ is about

$$|\boldsymbol{x}| = 2^{+9007199254740991} \cdot 10^{+308} \sim 10^{2120374989035370}.$$

Thus, in practice, almost all overflow or underflow problems are eliminated. Due to the ambiguity of the notation $(r, \boldsymbol{x}) \subseteq (r - s, 2^s \diamond \boldsymbol{x})$ the exponent $s \in \mathbb{Z}$ of the scaling factor 2^s can be chosen in such a way that, e.g. for a multiplication $(r_x, \boldsymbol{x}) \cdot (r_y, \boldsymbol{y}) \subseteq (r_x - s_x, 2^{s_x} \cdot \boldsymbol{x}) \diamond (r_y - s_y, 2^{s_y} \cdot \boldsymbol{y})$, the relations $2^{s_x} \cdot |\boldsymbol{x}| \sim 2^{s_y} \cdot |\boldsymbol{y}| \sim 10^{+153}$ are valid. In this case we have

$$(r_x, \boldsymbol{x}) \cdot (r_y, \boldsymbol{y}) \subseteq (r_x - s_x + r_y - s_y, (2^{s_x} \cdot \boldsymbol{x}) \diamond (2^{s_y} \cdot \boldsymbol{y}))$$

and because of $|(2^{s_x} \cdot \boldsymbol{x}) \diamond (2^{s_y} \cdot \boldsymbol{y})| \sim 10^{+306}$ an overflow is avoided and a maximum of about $153 + 324 = 467$ correct decimal digits can be achieved. Compared to the run time of $(2^{s_x} \cdot \boldsymbol{x}) \diamond (2^{s_y} \cdot \boldsymbol{y})$ the additional operations $r_x - s_x + r_y - s_y$ and $2^{s_x} \cdot \boldsymbol{x}, 2^{s_y} \cdot \boldsymbol{y}$ are negligible. Concerning the other operations $+, -, /$, similar considerations avoid overflows and lead to a maximum of accuracy. This will be demonstrated using the simple example of complex division.

In the new class `lx_interval` beside the basic arithmetic operations, a set of 42 real standard functions are implemented. Even for wide argument intervals $\boldsymbol{x}$ inclusions of $f(\boldsymbol{x})$ can be calculated. For rather tight intervals $\boldsymbol{x}$, with $|\boldsymbol{x}| \gg 1$ or $|\boldsymbol{x}| \ll 1$, optimal inclusions of rather sophisticated expressions are computable with high accuracy, even in cases where Computer Algebra Systems like Mathematica or Maple generate premature overflows or underflows. The new class `lx_interval` can be included additionally by a C-XSC program already using ordinary staggered intervals (C-XSC data type `l_interval`). Thus, critical code segments can use our modified staggered intervals (new data type `lx_interval`).

Along the same line of reasoning, extended complex staggered intervals $\boldsymbol{z}$ are defined by

$$\boldsymbol{z} = (r_r, \boldsymbol{x}) + i \cdot (r_i, \boldsymbol{y}), \quad i := \sqrt{-1}.$$

The basic arithmetic operations together with a set of 29 elementary complex transcendental functions are implemented in the new C-XSC class `lx_cinterval`. We will present some numerical examples to demonstrate the numerical quality of these functions.

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Complete Interval Arithmetic and its Implementation on the Computer

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Recently, the idea of standardizing interval arithmetic has gained considerable support. In this paper, a mathematically rigorous concept for the definition of interval arithmetic is presented. By means of option flags, alternative treatment of e.g. division by an interval containing zero may be enabled.

Let $I\mathbb{R}$ be the set of closed and bounded intervals of real numbers. Arithmetic in $I\mathbb{R}$ can be defined via the power set $I\!P\mathbb{R}$ (the set of all subsets) of real numbers. If divisors containing zero are excluded, arithmetic in $I\mathbb{R}$ is an algebraically closed subset of the arithmetic in $I\!P\mathbb{R}$, i.e., an operation in $I\mathbb{R}$ performed in $I\!P\mathbb{R}$ gives a result that is in $I\mathbb{R}$. Arithmetic in $I\!P\mathbb{R}$ also allows division by an interval that contains zero. Such division results in closed intervals of real numbers which, however, are no longer bounded. The union of the set $I\mathbb{R}$ with these new intervals is denoted by $(I\mathbb{R})$.

The paper shows that arithmetic operations can be extended to all elements of the set $(I\mathbb{R})$. On the computer, arithmetic in $(I\mathbb{R})$ is approximated by arithmetic in the subset (IF) of closed intervals over the floating-point numbers $F \subset \mathbb{R}$. The usual exceptions of floating-point arithmetic like underflow, overflow, division by zero, or invalid operation do not occur in (IF).

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Keywords: computer arithmetic, floating-point arithmetic, interval arithmetic, arithmetic standards

Bivariate Product Cubature Using Peano Kernels For Local Error Estimates

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To avoid the intrinsically embedded uncertainty problems that occur in the error estimates of multivariate integrators by pure floating-point arithmetic, we make use of product Gauss-Legendre rules to implement a self-validating subroutine for bivariate cubature over rectangular regions. In the subroutine, the local error estimation is done according to the Peano kernels theorem. That is, the local errors are estimated by the uniform norm of the partial derivatives of the integrands as well as the L_1-norm of the Peano kernels with respect to Gauss-Legendre rules. The uniform norm is then evaluated directly by interval arithmetic and automatic differentiation, and the L_1-norm can be derived by a root-finding process based on the extended interval Newton's method. A detailed discussion on the computation of Peano constants can be found in [1]. Based on the Peano kernels theorem, we generally have more than one choice to estimate a single local error. Thus, besides the commonly considered doubly adaptive strategies for region subdivision and local rules determination, it is possible to develop the third adaptive strategy for local error estimates. A practical way for performing triply adaptive quadrature is suggested in [2]. We extend the ideas discussed therein to our bivariate product cubature to enhance the computational effectiveness. In addition, the mechanism for active recognition of unreachable error bounds is also built in our subroutine. This makes the numerical computation of our software package robust and especially effective for strict accuracy requests. By different numerical examples, we show the uncertainty problems of a conventional integrator [3,4], and by numerical comparisons, we show that our algorithms generally require reasonable computational time and fewer function evaluations. Numerical examples have also shown that our routine can be superior to conventional approaches in efficiency, especially for integrands with oscillating factors. Besides, our approach can be relatively effective while conventional integrators encounter difficulties. It therefore can be served as a practical verification tool for automatic integration.

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Keywords: Adaptive cubature, product Gauss-Legendre rules, adaptive error estimates, Peano kernels.

Possibility of Objective Interval Uncertainty in Physics: Analysis

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In Newtonian physics, once we know the current state of the system, we can predict (at least in principle) all the future states of this system. In real life, measurements are never absolutely accurate, so we do not have the exact knowledge of the current state. However, the more accurate our measurements of the current state, the more accurate predictions we can make. The inaccuracy of the existing knowledge and of the resulting predictions can often be described in terms of interval uncertainty.

In quantum physics, we cannot predict the exact future state of a system such as a radioactive atom, we can only predict the probabilities of different future states. According to the modern quantum theory, if we know the exact initial state of the world, we can uniquely predict these probabilities. This means that the more accurate our measurements of the current state, the more accurate predictions of probabilities we can make. In practice, we can often only predict the intervals of possible values of the probability.

It seems reasonable to conjecture that for some real-life processes, there is no objective probability (= limit frequency), that for different subsequences, the corresponding frequencies can indeed take different values from a given interval. The analysis of such processes is given in [1].

How can we go beyond frequencies in this analysis? A common sense idea is that if an event has probability 0, then it cannot happen. This cannot be literally true since, e.g., for a uniform distribution on an interval $[0, 1]$, every number has probability 0 and thus, no number is random. According to Kolmorogov-Martin-Löf, we get a consistent definition of randomness if we only require that *definable* events of probability 0 do not happen [3]. Since there are only countably many defining texts and thus, countably many definable events, this leads to a consistent definition of a random object.

When we have a class $\mathcal{P}$ of probability distributions, we can similarly define an object to be $\mathcal{P}$-random if it does not belong to any definable event E for which $P(E) = 0$ for all $P \in \mathcal{P}$. In this talk, we show that for finite classes $\mathcal{P} = \{P_1, \ldots, P_n\}$, every $\mathcal{P}$-random object is random w.r.t. one of the probability measures P_i.

The main idea of this proof comes from [2]. If x is not random w.r.t. all P_i, then for every i, there exists a set $E_i \ni x$ with $P_i(E_i) = 0$. Then, $x \in E \stackrel{\text{def}}{=} \bigcap_{i=1}^{n} E_i$, and $P_i(E) = 0$ for all i.

We hope that this problem does not appear in the more physical interval-valued class $\mathcal{P}$.

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Keywords: random processes; interval uncertainty; physics; Kolmogorov complexity

A Practical Traffic Assignment Modeling Approach with Flexible Departure Time Choice and Travel Time Uncertainty

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In the transportation planning process, a city is divided into hundreds of traffic analysis zones. The Origin-Destination (O-D) matrix, which consists of the number of vehicles that depart from each zone and destined at other zones in the horizon year are estimated from projected land-use and demographic data. The road facilities are represented by a network of nodes and links, with finite capacities. Traffic assignment is the step that loads all the vehicles into the network in order to predict the spatial and temporal distribution of the traffic conditions (traffic volume, speed) across the network, subject to some equilibrium conditions. In practice, most of the planners use the static traffic assignment model which assumes that (1) there is only one O-D matrix, and the trip departure rates are the same throughout the day; (2) drivers select their routes with the fastest travel times. In reality, the trip departure rates vary by hours of the day and as a result, the traffic conditions also vary by hours of the day. The more advanced dynamic traffic assignment model attempts to account for this variation by the use of time-dependent O-D matrices and time-dependent shortest paths. However, the solution algorithm is computational intensive, and yet to be implementable in practice in a large network. This paper proposes a practical approach to solve the traffic assignment problem with time-dependent O-D matrices. Our approach has an inner loop that uses the familiar static traffic assignment algorithm to solve for the equilibrium link volumes given a fixed O-D matrix, and an outer loop that adjusts the users' trip departure times (and hence the O-D matrices) based on the inner loop's solutions. In addition, our traffic assignment algorithm takes into account drivers' route choice decisions due to travel time uncertainty. The inner and outer loops are solved iteratively until the time-dependent O-D matrices have reached a steady state. This approach has been implemented in the network in El Paso, Texas, to simulate the morning commute from 7:00 a.m. to 9:00 a.m. In this paper, we will demonstrate how the uncertainty in travel time has been modeled in the driver's route choice and departure time choice decisions, and study the convergence property of the solution approach.

A Global Optimization Algorithm for Intlab

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We present a new algorithm implemented in Intlab [5] for the unconstrained global optimization problem. The method itself is a simplified version of those much investigated in the past (as e.g. in [1] and [4]), which were first developed from the global optimization algorithm of the Numerical Toolbox [3]. Matlab is a natural environment for algorithm development and testing. We have recently completed a similar successful implementation in Matlab for the stochastic GLOBAL procedure [2]. We plan also in the case of the interval global optimization method to publish a complete numerical comparison to similar techniques.

The investigated algorithm uses only a subroutine calculating the objective function as information on the global optimization problem, i.e., the expression is not required. The procedure applies the gradient and the Hessian of the objective function, these are calculated by the automatic differentiation facility of Intlab.

The easy-to-use branch-and-bound type method applies the most common accelerating devices: the cutoff test, the concavity test, the monotonicity test, and the interval Newton step. Beyond natural interval extension (based on naive interval arithmetic), a simple centered (mean value) form inclusion function is also applied. Once the inclusion of the gradient is available, the intersection of these inclusion functions proved to be a good quality estimation of the range of the objective function. We use also multisection and advanced subdivision direction selection, albeit without those based on the pf^* heuristic algorithm parameter [1]. These later techniques will be inserted in the future: the present version is planed to be simple and easy to use.

We have completed a numerical test, and compared the efficiency and the results of the Intlab implementation to that of a C-XSC, BIAS, and Profil based procedure [4]. Algorithmically the two methods were more or less the same. The computational experiences (to be reported in detail at the conference) confirm that the new implementation is in several indicators (e.g. number of function, gradient and Hessian evaluations, number of iterations, and memory complexity) equivalent to that of the old one. The CPU time needed is as a rule by two order of magnitude higher for the Intlab version – as it is to be anticipated regarding the interpreter nature of Matlab. However, further vectorization coding changes in the algorithm may improve on that.

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Keywords: Global optimization, Intlab

Formal Methods for Rare Failures of Long Processes

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It is widely admitted that industrial processes contain flaws and they are allowed to fail. We describe a theory suitable for extremely rare failures of very long processes. This theory can be applied to hybrid systems modeling, for example an aircraft or a nuclear power plant on one side and its software on the other side. We are using PVS [1] and a previously published formal theory on random variables as such formal developments force explicit statement of all hypotheses and prevent incorrect uses of theorems [2].

Under the hypothesis that first order errors dominate, accumulated errors are sums of independent discrete and continuous variables. We derive a simple formula based on Lévy's and Markov's inequalities [3] that can be applied to any sequence of independent and symmetric random variables $\{X_n\}$ that admit second and fourth order moment bounded by $\mathbb{E}(X_i^2) \leq u^2/12$ and $\mathbb{E}(X_i^4) \leq u^4/80$, such as variables uniformly distributed over $[-u/2, u/2]$.

We bound the probability that the accumulated errors $S_i = \sum_{j=1}^{i} X_j$ were never above ϵ with

$$\mathbb{P}\left(\max_{1\leq i\leq n}(|S_i|) \leq \epsilon\right) \geq 1 - n\left(n + \frac{4}{5}\right)\frac{u^4}{72\epsilon^4}.$$

Quick highest order instantiation after a billion operations in single precision with a probability of failure below one against a billion shows that

$$\mathbb{P}\left(\max_{1\leq i\leq n}(|S_i|) \geq \epsilon\right) \lesssim u \qquad \text{leads to} \qquad \sqrt[4]{\frac{u}{72}} \lesssim \epsilon.$$

We conclude that about a fourth of the bits are significant where worst case analysis considers that no significant bit remains. Future developments will use Doob's original inequality [4] that follows a proof path very different form Doob-Kolmogorov inequality used in former developments. We may also prove the Central Limit Theorem and consider related work in validated numerics [5].

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A Statistical Method of Range Estimation for Embedded Applications

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Many embedded applications use fixed point arithmetic because embedded hardware do not implement floating point arithmetic for cost and efficiency reasons. In order to specify the fixed point arithmetics used in his design, a designer has to estimate the ranges of the internal variables. With this knowledge, he can obtain a trade-off between the cost, size, power and speed of his system. However, computing such a range is known to be difficult.

It can be observed that most of the embedded applications are digital signal processing and control applications which are generally iterative methods. Making use of interval or similar arithmetic [1, 2] in order to get an estimation of the range of such iterative methods does not give interesting results easily. The statistical methods offer an interesting way to get some information on the range simply.

The aim of such methods is to simulate several times with stimuli the application to be evaluated, to catch the values of the outputs and exploit some of their statistical properties in order to estimate their range.

Kim and Sung have proposed a method originally designed for estimating the range of variables of a C code [3]. In their approach, they examine the means, the standard deviations and the kurtoses of the studied internal variables. With this method, the width of the range of each variable is a simple function of those three parameters.

We propose here an other statistical method which requires less simulation than Kim & Sung's approach. If we consider the input stimuli as random independent inputs, it is then possible to consider the minima and the maxima of the outputs of each simulation as random variables. Assuming that these variables have a gaussian repartition, we built an estimator based on the student's test. The estimated range is then a function of the mean, the standard deviation, the number of simulation and the inverse of the student's T cumulative distribution function.

The use of our and Kim & Sung's method is also illustrated through several examples.

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Keywords: Range estimation, statistical methods, embedded applications

Analyzing the Relations between Interval-valued D-Implications, QL-Implications and Automorphisms

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Fuzzy set theory [1,2] is one of the key approaches for soft computing, leading to the design of flexible information processing systems, with applications in many different areas, such as control systems, decision making, expert systems, pattern recognition, etc. In fuzzy set theory, implication functions are usually derived from t-norms and t-conorms in several ways, e.g, S-implications, R-implications, QL-implications and D-implications. The importance of implications is not only because they are used in representing "If ... then" rules in fuzzy systems, but also because their use in performing inferences in approximate reasoning and fuzzy control. This is the main reason for searching many different models to perform this kind of operators.

Interval-valued fuzzy set theory aims at the integration of Fuzzy Theory and Interval Mathematics, and has been studied from different viewpoints (see, e.g., [3]). Lodwick [4] points out four ways to integrate fuzzy and interval approaches. One of them uses membership functions with intervals values, in order to model the uncertainty in the process of determining exact membership degrees with the usual fuzzy membership functions. In this paper, we adopt the approach used in our previous works (e.g., [5,6]), where interval extensions of fuzzy connectives are constructed as their interval representations, which considers both correctness (accuracy) and optimality aspects. In this approach, interval t-norms, interval t-conorms and interval fuzzy negations are defined in a primitive way, that is, as functions on $\mathbb{U} = \{[a, b] \mid 0 \leq a \leq b \leq 1\}$, satisfying conditions analogous to the respective punctual fuzzy connectives. It is shown in which condition these fuzzy interval operations coincide with the images of a respective punctual connective.

An interval fuzzy implication $\mathbb{I}$ is an *interval QL-implication* [5] whenever there are an interval t-conorm $\mathbb{S}$, an interval t-norm $\mathbb{T}$ and a strong interval fuzzy negation $\mathbb{N}$ such that $\mathbb{I}(X, Y) = \mathbb{S}(\mathbb{N}(X), \mathbb{T}(X, Y))$. However, if $\mathbb{I}(X, Y) = \mathbb{S}(\mathbb{T}(\mathbb{N}(X), \mathbb{N}(Y)), Y)$, then $\mathbb{I}$ is called an *interval D-implication* [6]. The aim of this work is to analyze the relationship between interval QL-implications, interval D-implications and interval automorphisms [5,6], studying several important properties that relate those concepts. In particular, we analyze under which conditions the main properties relating punctual D-implications and QL-implications [7] are still valid when we consider an interval-based fuzzy approach. The effects of the actions of interval automorphisms on interval D-implications and interval QL-implications are also discussed.

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Keywords: Interval QL-implication, interval D-implication, interval automorphism

Exact Numerics in a Categorial Framework

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We present the design and implementation of a static analysis framework, and its application to verified numerical computations based on the general theory of Abstraction Interpretation. Static analysis is the science of predicting, at program translation time, sound and computable approximations to runtime values and behaviours of a computer program. This work has been conducted in the OpenAxiom system, a strongly typed computer algebra system offering an advanced two-level type system for writing mathematical algorithms. Our work rests on two fundamental points: (1) principled and sound approximations of program semantics by Abstract Interpretation; and (2) use of advanced type system for enabling semantics-based program transformation. Finally, we show applications of this framework to computational geometric predicates.

A popular approach to the *exact computation* paradigm is the use of arithmetic filters [3,4] for validated computation, e.g. in computational geometric predicates. The spectrum of arithmetic filters is essentially characterized by two extrema: *static filters* (where error bounds are known at compile time), and *dynamic filters* (where error bounds and approximations are computed at run time). In between are so-called *semi-static filters* with varying degree of mixture between static and dynamic filter properties. Our contribution is a semantics-based program transformation framework for supporting exact computations, developed in the OpenAxiom computer algebra system. Early versions of our framework have been successfully applied to the field of algorithmic differentiation [7].

Abstract Interpretation is a general theory for approximating the behaviour of dynamical systems, in particular the runtime semantics of computer programs [1,2]. Beyond its traditional area of application — data flow analysis, and other optimizations in the field of compiler construction — Abstract Interpretation has been successfully applied to various kinds of static analysis and program transformations, in particular in proving absence of runtime errors in programs written in the C programming language [5].

OpenAxiom is an open source platform for symbolic, algebraic, and numerical computations. It offers an interactive environment, an expressive programming language, a compiler, a large set of mathematical libraries of interest to researchers and practitioners of computational sciences. OpenAxiom is a descendent of AXIOM, a research project at IBM Research, later commercialized by NAG and now open sourced. Unlike most popular computer algebra systems, OpenAxiom is strongly typed. This means that every expression has a type that describes permitted operations. Values belong to *domains of computations*. Domains of computations implement value representations and routines to operate on values. They are structured by specifications called *categories* in the OpenAxiom community. Categories help manage complexities in expressing generic algorithms involving semantically rich mathematical structures. Both categories and domains can be parameterized by categories, domains, and values.

Our framework builds upon the key property that domains can be instantiated at run time, values can migrate from one domain of computation to another without additional costs, and that OpenAxiom performs overload resolution of operators based on the types of the arguments and attributes associated with those types as described by their structuring categories. This, and the typed abstract syntax tree library we developed for algorithmic differentiation [7], enables a tool for 'instantiating' the same program component as either a static filter, or a dynamic filter, or a combination of both.

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Keywords: Verified Numerics, Program Tranformation, Abstract Interpretation

Convex Decomposition of Interval-Based Octrees

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Constructive solid geometry models (CSG-models), boundary representation models (B-Rep-models) and tessellations (e.g. octrees) are the most widely used representations of geometric objects on the computer. The idea of the octree data structure is to recursively subdivide a box including objects in a three-dimensional space into eight disjoint boxes until the required closeness to the objects is reached [1]. The utilization of interval arithmetic in the context of geometric modeling guarantees on the one hand, that all points of the object are enclosed within its interval-based representation and on the other hand, that exact results of geometric operations executed on this object representation are always included in the result intervals. In contrast to the CSG- or B-Rep-model, the octree-encoded object representation is particularly suitable for dealing with interval arithmetic. An axis-aligned box as the underlying basic entity of the tree can be directly stored as an interval vector. If the geometry of the primary object is known, e.g., its surface is described by a union or intersection of areas defined by implicit functions then we can apply the test for classifying points in space as inside, on the boundary or outside the object to be performed at once to the whole axis-aligned box using interval arithmetic.

A feasibility study regarding accuracy of operations on the interval-based structure is still an important pending goal of the model analysis. In the case of an axis-aligned octree, all boxes have as vertices machine numbers that are multiples of a power of two. This fact enables us to categorize geometric operations that can be realized exactly for the tree representation. The decomposition of an octree into simpler components ranks among logical operations on the structure and thus it belongs to the category of exact operations.

In this talk, a new approach for an accurate decomposition of an interval-based octree data structure into convex parts is presented. The method is based on the reliable convex hull algorithm suggested in [2] to estimate the remaining concavity of the object parts, as well as on the algorithm for connected component labeling introduced by Samet [1]. In addition, a kind of an inverse concept of extreme vertices to this one used in [2] has been adapted. The separation planes are calculated by weighting several criteria by factors to optimize the achieved result. In the case of an octree, the convex components describe rectangular axis-aligned volumes that can be stored as interval vectors. The decomposition yields a data compression resulting from the number reduction of interval vectors needed to approximate the object. Thus the proposed new method can be used to speed up geometric computations, like collision detection or distance calculation.

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Keywords: Reliable solid modeling, octree data structure, convex decomposition, accurate algorithms

Verified Solution and Propagation of Uncertainty in Physiological Models

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Physiological models are used to simulate the dynamics of the human body, especially in cases where experimenting on humans is not a viable option. Further, simulations with an ordinary differential equations model can allow for a large number of numerical experiments to be performed, by adjustment and control of specific model parameters. These models may need to be tested over a range of parameter values, since in many cases these parameters are not known with complete certainty, though some knowledge of the probabilistic distribution of the parameter values may be available.

In this presentation, we demonstrate a method for finding verified solutions of nonlinear ODE models in physiology, thus computing rigorous bounds on the trajectories of the state variables, based on the ranges of the uncertain parameters. The method is based on the general approach described by Lin and Stadtherr [1], which is based on the use of an interval Taylor series to represent dependence on time, and the use of Taylor models to represent dependence on uncertain parameters and/or initial conditions.

We also demonstrate in this presentation an approach for the propagation of uncertain probability distributions in one or more model parameter and/or initial condition. Assuming an uncertain probability distribution (p-box) for each parameter and/or initial condition of interest, we use a method, based on Taylor models and recently described by Enszer et al. [2], that propagates these distributions through the dynamic model to the state variables. As a result, we obtain a p-box describing the probability distribution for each state variable at time intervals of interest. As opposed to a traditional Monte Carlo simulation approach, in which it is impossible to sample the complete parameter space with a finite number of trials, this Taylor model method provides completely rigorous results.

As test problems, we use two physiological models. The first is a simulation of starvation that models the mass of the human body over time given uncertain metabolic rates [3]. This model explicitly assumes probability distributions for the parameters of interest. The second model simulates the metabolism of glucose in diabetic patients [4]. In both problems, comparisons are made with results obtained from Monte Carlo analysis.

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Keywords: Ordinary differential equations, Interval analysis, Probability bounds analysis, Physiology

Verified Computation with Probability Distributions: Applications to Engineering and Superfund Contamination Sites

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Engineers use probability theory ubiquitously in diverse calculations such as risk analyses and stochastic modeling. However, when data are scarce or scientific knowledge is incomplete, probability estimates may not be very good. When the potential consequences of miscalculation are serious, it is important to assess the reliability of probabilities. In the past, when probability theory has been used to make calculations, analysts have routinely assumed (i) probabilities and probability distributions can be precisely specified, (ii) events and numerical variables are all independent of one another or at least that the dependencies among them are well specified, and (iii) model structure is known without error. For the most part, these assumptions have been made for the sake of mathematical convenience, rather than with any empirical justification. And, until recently, these assumptions were pretty much necessary in order to get any answer at all.

Several researchers have suggested characterizing the uncertainty about probabilities with a bounding analysis that uses *probability intervals* (i.e., subranges from [0,1]) and ordinary interval analysis. This approach can rigorously enclose uncertainty about a probability value, and it is sometimes a practical approach, but it can become clumsy and does not have the delicacy required for many kinds of calculations. A more practical structure for such uses is the probability box, or *p-box*, which consists of interval-like upper and lower bounds around a cumulative distribution function. Probability bounds analysis is a collection of methods for projecting p-boxes through mathematical expressions. These methods allow us to compute bounds on probabilities and probability distributions that are guaranteed to be correct even when one or more assumptions is relaxed or completely removed. In many cases, the bounds obtained are mathematically best possible, which means that tightening them would require additional empirical information.

These new methods have already been applied to many practical problems in engineering and environmental science. In human health risk analyses conducted as part of the assessments for Superfund sites in the United States, probability bounds analysis has been used to account for uncertainty in the estimates of human exposures to the environmental pollution. P-boxes have also used to bound uncertainty about global climate change and about the number of species that have gone extinct due to anthropogenic impacts. They've also been used to relax untenable assumptions in estimating the reliability of engineered structures such as dikes. The methods have been used in modeling the temporal evolution of contaminant plumes in groundwater, and a project will soon be underway to extend their application to computational fluid dynamics models of plumes in the atmosphere. The methods also have obvious applications in finance computations and wherever

there is a collision of incomplete knowledge about processes that involve natural variation across time or space or among individuals.

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Keywords: p-boxes; probability bounds analysis; imprecise probabilities; model uncertainty

Solving ODEs via New Implicit Methods and Jacobian-Free Newton-Krylov Solver

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There are a variety of approaches available for numerical solution of stiff and non-stiff ordinary differential equations (ODEs) arising from engineering and physics, including linear multi-step, explicit and implicit Runge-Kutta, Taylor and extrapolation methods. Stiff differential equations are equations which are ill-conditioned in a computational sense.

In the last 30 years or so, numerous works have been focusing on the development of more advanced and efficient methods for stiff problems. Most of these improvements in the class of linear multi-step methods have been based on backward differentiation formula (BDF), because of its special properties. These methods are A-stable or A(α)-stable. But, many important classes of practical problems of applied mathematics, engineering and computational science do not require stability on the entire left half-plane of complex plane [4]. On the other hand, stiff equations are problems for which explicit methods don't work [4]. Thus, solving stiff systems of ordinary differential equations (ODEs) requires implicit formulas having reasonable stability regions, good accuracy and higher order. Also, it is to be noted that the effective evaluation of such formulas is absolutely fundamental.

In this paper, we are going to get new one-step methods which are potentially good numerical schemes for the solution of first- order stiff ordinary differential equations (ODEs) of the form

$$y' = f(x, y), \qquad y(a) = y_0, \tag{1}$$

where $x \in R$, $y \in R^m$ and $f \in R^{m+1}$.

These methods are generalized single-step methods (GSM) based on Newton-Cotes integration formulas [7] of the form

$$y_{n+1} = y_n + h\left[\beta_n f_n + \sum_{i=1}^{k} \beta_i \hat{f}_{n+v_i} + \beta_{n+1} f_{n+1}\right], \tag{2}$$

where

$$\hat{f}_{n+v_i} = f(x_{n+v_i}, \hat{y}_{n+v_i}), \qquad x_{n+v_i} = x_n + v_i h, \qquad 0 < v_i < 1,$$

for $i = 1, ..., k,\ k = m - 1,\ m = 5$ and 6. We note that β_i's are parameters which must be chosen appropriately. These methods are implicit and have at least four off-step points. In fact, we are

using two step-points and at least four off-step points which are between those step-points. At these off-step points we are using a sixth-order explicit one-step method of the form [2]

$$\hat{y}_{n+v_i} = y_n + h_i \left(f_n + h_i \left(\frac{f_n^{(1)}}{2} + h_i \left(\frac{f_n^{(2)}}{6} + h_i \left(\frac{f_n^{(3)}}{24} + h_i \frac{f_n^{(4)}}{120} \right) \right) \right) \right) + \omega_n, \tag{3}$$

where

$$\omega_n = f_n^{(4)} \left(\exp(h_i z_n) - 1 - h_i z_n \left(1 + h_i z_n \left(\frac{1}{2} + h_i z_n \left(\frac{1}{6} + h_i z_n \left(\frac{1}{24} + h_i \frac{z_n}{120} \right) \right) \right) \right) \right) \Big/ z_n^5,$$

$z_n = \dfrac{f_n^{(5)}}{f_n^{(4)}}$, $h_i = v_i h$, $0 < v_i < 1$, $i = 1, ..., k$, $k = m - 1$, and, $m = 5$ or 6. In method (3), $f_n = f(x_n, y_n)$ where $f(x, y(x))$ has desired total derivatives, $f_n^{(k)}$ is the k^{th} order derivative of $f(x, y(x))$, $x_n = nh$ and h is stepsize.

Order of truncation error of new generalized single-step methods (GSM) are obtained and Stability domains of them also discussed showing that our new methods have higher orders and wide absolute stability regions for solving some stiff systems of $ODEs$. Numerical results are presented for three test problems and compared with those of standard BDF schemes. Saving CPU time is very important when stiff system of ODEs are beeing solved by numerical methods. CPU time of the new GSM has also been obtained and compared with those of standard existing BDF schemes by using MATLAB V6.5.1 showing that there is saving of CPU time. Thus, these new numerical methods are suitable for solving first-order stiff systems of ODEs numerically. Newton-Krylov method [3] and automatic LU factorization [5] are used in the present paper which are needed for our implicit methods.

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Keywords: Stiff and non-stiff ODEs, A-stability, A(α)-stability, BDF.

Theory of Hyper-Random Phenomena

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Most physical phenomena (electrical, electromagnetic, mechanical, acoustics, nuclear, and others) are of indeterminate type. Usually, different stochastic methods based on classic probability theory are used to describe them. However, possibilities of such methods are limited. Serious problems occur, when observation conditions are changed in space or time and it is impossible to determine the statistical regularity, even by using a large experimental sample size.

Changing conditions are everywhere. It is impossible to imagine any real event, magnitude, process or field in absolutely fixed conditions. All mass measurements are conducted in the variable conditions, only partially controlled.

Difficulties and often impossibility to use the probability theory in many cases stimulate the development of new approaches, in particular connected with fuzzy technologies, neural network, chaotic dynamical systems, and others. The new theory of hyper-random phenomena, the basis of which are presented below, can be included in this list too.

The aim of the presentation is to review the original author's researches published in a number of articles and combined in the monograph [1].

Hyper-random phenomena can be defined by a tuple $(\Omega, \mathcal{F}, G, P_g)$, where Ω and $\mathcal{F}$ are the set of simple events and the Borel field respectively (as in the case of the probability field), G is the set of the conditions $g \in G$, and P_g is the probability distribution corresponding to a condition g.

Any hyper-random phenomena (events, variables, functions) can be regarded as a set (family) of random subsets. Every subset is associated with a fixed observation conditions. The probability measure is determined for every element of each subset; however, the measure is not determined for the subsets of the set.

Modern theory of hyper-random phenomena includes:

- mathematical definition of the main hyper-random concepts, in particular, of hyper-random event, hyper-random variable, and hyper-random function;
- formalization of series of concepts related to hyper-random phenomena: mean-square convergence of the sequences of hyper-random variables and hyper-random functions, stationarity and ergodicity of the hyper-random functions, hyper-random sample, etc.;
- description methods for hyper-random events and for scalar, vector, real, and complex hyper-random variables and hyper-random functions;
- special description methods for stationary and ergodic hyper-random functions;
- Markov hyper-random model theory;
- emerging methodology of hyper-random estimates, convergence conditions of hyper-random estimates, limit theorems, laws of large numbers;

- point and interval estimation methods for variables and functions described by hyper-random models, and so on.

The hyper-random approaches make it possible to model different types of real physical objects and to provide estimates of these quantities in situations when the statistical properties of the objects and of the observation conditions can change unpredictably.

A hypothesis have been proposed (called the *hyper-random hypothesis*) that all real physical phenomena (with the possible exception of fundamental physical constants) are of hyper-random type, i.e., these phenomena are not statistically stable: their statistical characteristics can (unpredictably) change. It has been shown that hyper-random quantities cannot be estimated in a statistically consistent way, in the sense that even when the sample size increases (and tends to infinity), the estimate inaccuracy does not tend to 0.

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Keywords: random; hyper-random; phenomenon; probability; statistics

Interval Multivalued Inverse Functions: Algorithms and Applications

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Given the relation $y = \cos x$, where x lies in the interval $[10, 14]$, interval arithmetic will readily allow us to compute the possible values for y by considering the monotonic subdomains of the cosine function over $[10, 14]$: $y \in [\cos 10, 1] \approx [-0.84, 1]$. On the other hand, what is the possible domain for an unknown x if the domain for y is $[-0.3, 0.2]$? Most interval arithmetic libraries will fix it at $[\operatorname{acos} 0.2, \operatorname{acos} -0.3] \approx [1.36, 1.87]$ because they consider branch cuts of the multivalued inverse cosine to return principal values in the domain $[0, \pi]$ only. Now, what if we know that x lies in the domain $[20, 26]$? The aforementioned inverse cosine interval function would not be of much help here, while considering a *multivalued inverse cosine* would permit restricting the domain of x to $[6\pi + \operatorname{acos} 0.2, 8\pi - \operatorname{acos} 0.2] \approx [20.22, 23.77]$.

Such a use of relations between variables together with domains of possible values to infer tighter consistent domains is the core principle of *Constraint Programming* [2,3]. Since Cleary's seminal work [1] on *relational arithmetic* for Logic Programming languages, interval multivalued inverse functions have been repeatedly used in algorithms of increasing sophistication to solve systems of (in-)equations over real-valued variables.

Using these functions as both a starting and rallying point, we present an overview of these constraint programming algorithms, and we draw parallels with classical numerical algorithms (most notably Gauss-Seidel). The implementation of interval multivalued inverse functions in the *gaol* C++ library is also discussed.

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Inner and Outer Approximation of Functionals Using Generalized Affine Forms

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We propose a method for the joint computation of inner and outer approximations of the range of vector-valued set-theoretic functionals, defined by arithmetic expressions, intersections, unions and least fixpoints.

The context is that of static analysis for the validation of programs, where we want to synthetise automatically guaranteed approximations of the possible range of variables at control points of the program, for a possibly infinite set of executions. The functionals involved are the ones characterizing these ranges of variables, at each control point, or, said in a different manner, characterizing the invariant sets under the action of the discrete dynamical system defined by a program. One salient feature is that inputs and parameters of programs to analyse are given in possibly large sets, and there may be a large number of them.

In guaranteed numerical methods, the price you pay for being guaranteed is potential overestimation. Indeed, an unexpectedly large range of values for a variable can be due either to a "bug" in the program analyzed, or to an overestimation due to the outer approximation method. A joint computation of inner and outer approximations allows us to answer this question and express the quality of the approximation. Moreover, we will show that this joint computation also allows us to generate worst-case scenarios, i.e. actual values for inputs and parameters that lead to an extremal (or close to extremal) output of the program.

Building on work [1] by Goldsztejn and al. on Kaucher arithmetic for generalized intervals [2] and its interpretation with modal intervals, and extending the first ideas we proposed in [4], [5], we describe a new approximation scheme based on affine forms [3]. Using the generalized mean-value theorem proposed in [1], we derive affine forms but with interval coefficients, that can be interpreted in two different manners, giving respectively an inner and an outer approximation. We also propose union and intersection operations on these forms that allow for precise computations of least fixed points, or invariant sets.

We will give some examples, both exemplifying some results we get in the scope of static analysis of programs, and comparing our results to the ones of [6]: we show in particular that our inner-approximations allow to express relations between values of specific subsets of variables of the program.

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Keywords: inner-approximation, affine arithmetic, validation by static analysis

Accurate Simple Zeros of Polynomials

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We examine the local behavior of the Newton's method in floating point arithmetic for the computation of a simple zero of a polynomial assuming that a good initial approximation is available. We allow an extended precision (twice the working precision, namely twice the number of digits of the working precision) in the computation of the residual. For that we use the compensated Horner scheme (`CompHorner`) which satisfies the following error bound

$$|\texttt{CompHorner}(p,x) - p(x)| \leq \texttt{eps}|p(x)| + \gamma_{2n}^2 \tilde{p}(x),$$

where $p(x) = \sum_{i=0}^{n} a_i x^i$, $\tilde{p}(x) = \sum_{i=0}^{n} |a_i||x|^i$, and `eps` is the relative rounding error (for example $\texttt{eps} = 2^{-53}$ in IEEE 754 double precision).

We use the following accurate Newton's algorithm.

Algorithm 1. *Accurate Newton's method*

$$x_0 = \xi$$
$$x_{i+1} = x_i - \frac{\texttt{CompHorner}(p, x_i)}{p'(x_i)}$$

We assume that we already know that the root we are looking for belongs to $[a, b]$ with $a, b \in \mathbb{R}$ and we denote $\beta = \max_{x\in[a,b]} |p'(x)|$.

We prove that, for a sufficient number of iterations, the zero is as accurate as if computed with twice the working precision.

Theorem 1. *Assume that there is an x such that $p(x) = 0$ and $p'(x) \neq 0$ is not too small. Assume also that*

$$\texttt{eps} \cdot \mathrm{cond}(p, x) \leq 1/8 \text{ for all } i,$$

where $\mathrm{cond}(p, x) = \tilde{p}(|x|)/|p(x)|$. *Then, for all x_0 such that*

$$\beta \cdot |p'(x)^{-1}| \cdot |x_0 - x| \leq 1/8,$$

Newton's method in floating point arithmetic generates a sequence of $\{x_i\}$ whose relative error decreases until the first i for which

$$\frac{|x_{i+1} - x|}{|x|} \approx \texttt{eps} + \gamma_{2n}^2 \,\mathrm{cond}(p, x).$$

We provide numerical experiments confirming this. Concerning the number of iterations needed for the accurate Newton's algorithm, it is not clear whether it is the same as the classic Newton's algorithm.

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Keywords: zeros of polynomials, Newton's method, condition number, floating point arithmetic

Interval Arithmetic on the Cell Processor

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The Cell processor is a new processor [2], designed by IBM, Sony and Toshiba, with an innovative architecture based on 8 Synergistic Processor Elements on the same chip. Each SPE contains a synergetic processing unit (SPU), a local memory (256KB of memory for the code and the data) and a memory flow controller. The SPU [1] is composed of a 4-way SIMD single precision FPU (SpSPU) and a 1-way SIMD double precision (DpSPU). Today, the peak rate is around 200 Gflops. Each SpSPU can perform 25.6 GFlops whereas DpSPU can only do 1.8GFlops. But SpSPU has only the rounding mode toward zero and no underflow and overflow whereas the DpSPU is fully IEEE 754 compliant.

In order to deal efficiently with interval arithmetic [3] with only rounding mode toward zero, we discuss different ways to represent intervals and compare them on the SpSPU and on the DpSPU.

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Keywords: Cell processor, interval arithmetic, rounding toward zero

Constructive A Priori and A Posteriori Error Estimates for Bi-Harmonic Problems

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For the numerical verification method of solutions for nonlinear fourth order elliptic problems, it is important to find a constant in the constructive a priori and a posteriori error estimates for the finite element approximation of linear fourth order elliptic problems. We show how to compute these constants by verified computational techniques using the Hermite spline functions. Several numerical results which confirm the actual effectiveness of the method are presented.

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Keywords: Constructive a priori error estimate, bi-harmonic problem

Block Floating Point Interval ALU for Digital Signal Processing

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Numerical analysis on real numbers is performed using either point-wise arithmetic or interval arithmetic. Today, interval analysis is a mature discipline and finds use not only in error analysis but also control applications such as robotics. Using current hardware architectures that have no support for performing interval arithmetic has resulted in poor execution rates when operating on interval based arithmetic. This has provided a strong motivation for developing an architecture to perform interval operations efficiently. Despite the fact that floating-point computation based interval architectures have been proposed [1,2], we deem fixed point computation based architectures, such as the dedicated interval arithmetic and logic unit (I-ALU) [3], more feasible for implementation since fixed point digital signal processors provide comparatively lower price per chip, better speed and power efficiency over their floating point counterparts. We note, however, that the I-ALU is prone to unreliability owing to overflow errors resulting from the small dynamic range offered by fixed point.

In this paper, we present a solution to the problem in the form of a fixed point interval ALU that utilizes the concept of Block Floating Point (BFP) [4] to attain a higher dynamic range for interval as well as point-wise computations. We add block floating point support to the ALU in the form of special instructions such as Exponent Detection and Normalization that aid the change of the dynamic range of the input. We retain the skeleton of the architecture from the work of [3], comprising of two independent modules that compute the upper and lower endpoints of the interval result simultaneously. However, each of these modules is provided with additional logic that performs Conditional Block Floating-point Scaling (CBFS) on the output. CBFS is implemented by automatically scaling the result down by a factor of 2 if overflow is detected. We expand upon the utility of this architecture by providing the capability to perform point-wise operations in addition to interval operations. We add one more block at the output of these modules to perform appropriate synchronization and rounding depending upon the type of operation performed by the ALU. We conclude this paper by characterizing the performance of our hardware as the number of output samples processed per second, expressing it as a function of the number of overflows and the fastest clock that can be applied to it.

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Keywords: fixed point, interval, digital signal processing, block floating point

Computing Condition Numbers with Automatic Differentiation

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Condition numbers are mathematical quantities widely used either for measuring the sensitivity of the solution of a problem to perturbations of the input, or, after a backward error analysis, for deducing first-order error bounds on the computed solution.

In this talk, we address the question of effectively computing such numbers for basic algebraic problems like inverting and factoring an $n \times n$ real matrix A. Viewing each of these problems as a map $f : \mathbb{R}^p \to \mathbb{R}^q$ with $p \leq n^2$ and $q = O(n^2)$, condition numbers can be expressed in terms of a norm of the input A, a norm of the exact solution $f(A)$, and a norm of the Jacobian matrix J of f (see for example [2]).

Using this approach, we first show how to recover the classical formulas for matrix inversion [1]. For example, using the Frobenius matrix norm $\|\cdot\|_F$ and taking $f(A) = A^{-1}$, we get $J = -A^{-t} \otimes A^{-1}$ and the condition number

$$\mathrm{cond}_F(f, A) := \lim_{\varepsilon \to 0} \sup_{\|\Delta A\|_F \leq \varepsilon \|A\|_F} \frac{\|f(A + \Delta A) - f(A)\|_F}{\varepsilon \|f(A)\|_F}$$

is then equal to $\|A^{-1}\|_2^2 \|A\|_F / \|A^{-1}\|_F$.

Using automatic differentiation makes it possible to compute condition numbers for which the Jacobian matrices are either not given explicitely, or given by formulas more complicated than the above one. Those numbers can furthermore be significantly smaller than the bounds usually found in the literature. For example, let $f : A \mapsto R$, where R is the upper triangular factor in the QR-factorization of A. It turns out that $\mathrm{cond}_F(f, A) = \|J\|_2$ and, using the "max norm" $\|A\|_M = \max_{i,j} |a_{i,j}|$, that $\mathrm{cond}_M(f, A) = \|J\|_\infty \|A\|_M / \|R\|_M$. Taking for instance

$$A = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & \alpha \end{bmatrix}, \quad \alpha = 10^{-5},$$

yields $\mathrm{cond}_F(f, A) = 1.732050\ldots$ which is more than 10^5 times smaller than the upper bound $\|R\|_F \|R^{-1}\|_F = 599999.000019\ldots$ used in classical normwise sensitivity analyses [3]. For the "max norm", computations can be done exactly and we get $\mathrm{cond}_M(f, A) = (1 + 10^{-5})\sqrt{6}$ while $\|R\|_M \|R^{-1}\|_M = 10^5 \sqrt{6}$.

We will show in this talk how this general approach has been implemented using automatic differentiation for computing Jacobian matrices. The result is a C++ toolbox for effectively computing various condition numbers like those in the above examples. Different arithmetics can be used interchangeably, like mutiple precision floating-point interval arithmetic (MPFI) or rational arithmetic (GMP). The toolbox can be used for computing tight enclosures of condition numbers

or even exact values (typically when the problem can be solved exactly with rational arithmetic). We will present a set of experiments with this toolbox that involve unstructured condition numbers as well as their structured counterparts for Toeplitz, Sylvester, Vandermonde and Cauchy matrices.

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Keywords: condition number, automatic differentiation, arithmetics.

Dynamics with a Range of Choice

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Mathematical setting for discrete dynamics is a state space, X, and a map $S : X \to X$ (the evolution operator) which defines the change of a state over one time step. Dynamics with choice, as we define it in [2], is a generalization of discrete dynamics where at every time step there is not one but several available maps that can transform the current state of the system. Many real life processes, from autocatalytic reaction systems to switched systems to cellular biochemical processes, exhibit the properties described by dynamics with choice. We are interested in the long-term behavior of such systems. In [2] we studied dynamics with choice with a finite number of available maps, S_0, $S_1, \dots, S_{N-1}$. The orbit of a point $x \in X$ then depends on the infinite sequence of symbols from the set $\mathcal{J} = \{0, 1, \dots, N-1\}$ encoding the order of maps S_j applied at each step. Denote by Σ the space of all one-sided infinite sequences of symbols from $\mathcal{J}$ and denote by σ the shift operator that erases the first symbol in sequences. We define the dynamics on the state space X with the choice of the maps S_0, $S_1, \dots, S_{N-1}$ as the discrete dynamics on the state space $\mathfrak{X} = X \times \Sigma$ with the evolution operator $\mathfrak{S} : (x, w) \mapsto (S_{w(0)}(x), \sigma(w))$, where $w(0)$ is the first symbol in the sequence w.

In this paper we address the case when there is possibly a continuum of available maps parameterized by points from the interval $[0, 1]$ or any metric compact $\mathcal{J}$. (Think of a system of equations with parameters, where each parameter may change from step to step while staying within a prescribed interval.) We say that there is *a range of choice*. We give mathematical description of dynamics with a range of choice and prove general results on the existence and properties of global compact attractors in such dynamics. One of practical consequences of our results is that when the parameters of a nonlinear discrete-time system are not known exactly and/or are subject to change due to internal instability, or a strategy, the long term behavior of the system may not be correctly described by a system with "averaged" values for the parameters. There may be a Gestalt effect.

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Keywords: Global Attractors, Discrete-time dynamics, Symbolic Dynamics.

Interval-based Analysis of Large SMP/GI/1 Queues

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Semi-Markov processes (SMPs) are known and adequate models for correlated data traffic in service-integrated communication networks [1]. Methods to determine the parameters of a SMP model of an arrival process are described in [2]. Using these methods, original video traffic as well as aggregated traffic from different types of sources is described by SMP models in a small state space, preserving the autocorrelation function of the original data series. To increase the accuracy of these models, however, more states may be considered in the underlying Markov chain. Aggregated traffic from several sources may furthermore be given as a superposition of semi-Markovian models, thus resulting in a consequently larger state space. Using known techniques for an interval-based analysis studied in previous work [3], a verification of these large is not feasible in every case.

In this paper, we propose improvements to these known methods for the verified analysis of SMP/GI/1 queues. On the one hand, using the new techniques, we are able to yield more accurate results for small SMP models described previously in literature. On the other hand, it is now feasible to analyse larger SMP models.

These improvements consist of a modified polynomial factorization technique. As an alternative to finding the roots of the characteristic polynomial using verified algorithms, we consider this as an instance of the polynomial eigenvalue problem. This way, we can apply dedicated verified eigenvalue algorithms included, for instance, in INTLAB [4]. Further improvements to the polynomial factorization are considered and discussed. Additionally, we present an application of the successive over-relaxation (SOR) technique to the verified Wiener-Hopf factorization, which is determined using a SMP extension of the Grassmann-Jain algorithm [5]. This way, the the speed of convergence is improved, resulting in faster analysis and the ability to study larger examples.

We evaluate these improved methods on a set of examples described previously in literature as well as on detailed models of original H.264 video traffic. All methods discussed are to be included in our integrated toolkit for modeling and interval-based analysis of correlated data traffic, *InterVerdiKom* [6].

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Keywords: Interval arithmetic, Semi-Markov processes, Wiener-Hopf factorization, Polynomial Eigenvalue Problem

Numerical Verification of Solutions for Boundary Value Problems with High Accuracy by Using Spectral Method

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In this report, we discuss a priori error estimates of the spectral approximation for elliptic boundary value problems using Legendre polynomials. As a numerical example, we compute a weak solution of Emden equation with very accurate and guaranteed error bounds by computer assisted proof.

The spectral method is known as an approximate method of solutions based on the orthogonal base functions on concerning domain, and in general, it has a possibility to obtain a highly precise approximate solution than finite element method or finite difference method. While, in the finite element method, the residual norm decreases by polynomial order of the mesh size, in the spectral method, it usually decreases with exponential order of the number of base functions. As for base functions used in the spectral method, it is experimentally known that the approximation accuracy will highly depend on boundary conditions. For example, the trigonometric Fourier bases are good for the periodic boundary condition and Legendre or Chebyshev polynomials are good for Dirichlet conditions.

Let S_N denote the finite dimensional subspace of H_0^1 generated by Legendre polynomials with degree less than N, and define the H_0^1-projection $P_N : H_0^1 \to S_N$ by

$$(u - P_N u, v_N)_{H_0^1} = 0, \quad \forall v_N \in S_N.$$

In this talk, we present some constructive a priori estimates of the error operator $I - P_N$, where I means the identity map on H_0^1, by using the orthogonality and the recurrence formula of Legendre polynomials. Similar kind of a priori error estimates, not constructive, are given in [2].

In numerical examples, we illustrate some computational results for the Emden equation with homogeneous Dirichlet boundary condition, by using the computer assisted proof technique presented in [1]. As shown in the talk, the verification result using Legendre polynomials is very accurate, which implies that we could prove the existence of an exact solution very close to the approximation solution by our method. Moreover, we will also verify a fairly large non-existential domain in which there are no solutions at all.

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Keywords: spectral method, Legendre polynomial, a priori error estimate, numerical verification method, computer assisted proof

Asymmetric (Libertarian) Paternalism: Explanation Based on Decisions Under Interval Uncertainty, and Possible Applications to Education

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In the traditional approach to decision making (see, e.g., [1]), the decision maker's preferences $A_1, \ldots, A_n$ can be characterized by their "utility values" $u(A_1), \ldots, u(A_n)$, so that an alternative A_i is preferable to the alternative A_j if and only if $u(A_i) > u(A_j)$. So, unless the two alternatives A_i and A_j have the exact same utility value $u(A_i) = u(A_j)$, we have two possibilities:

- either $u(A_i) > u(A_j)$, i.e., the alternative A_i is better,
- or $u(A_j) > u(A_i)$, i.e., the alternative A_j is better.

In the first case,

- if we originally only had an alternative A_i, and then we are adding the alternative A_j, then we stick with A_i;
- on the other hand, if we originally only had an alternative A_j, and then we are adding the alternative A_i, then we switch our choice to A_i.

Similarly, in the second case,

- if we originally only had an alternative A_j, and then we are adding the alternative A_i, then we stick with A_j;
- on the other hand, if we originally only had an alternative A_i, and then we are adding the alternative A_j, then we switch our choice to A_j.

Interestingly, in the actual tests of the above experiment, human decision makers do not follow this seemingly rational behavior; see, e.g., [2,6]. Specifically, they exhibit "inertia", the desire not to change an alternative.

We show that this seemingly irrational behavior can be explained if we take into account that decision makers only know the utility value of different outcomes with interval uncertainty $[\underline{u}(A_i), \overline{u}(A_i)]$. In this case, a decision maker switches to the new alternative A_j only if it is guaranteed that the new alternative is better, i.e., that $\underline{u}(A_j) \geq \overline{u}(A_i)$.

The rationality of inertia under uncertainty can be illustrated on the example of a similar situation: how a mobile robot makes decisions about its motion.

In the traditional control, we make decisions based on the current values of the quantities. Measurement noise leads to random deviations of the robot from the ideal trajectory – shaking and "wobbling". A natural way to avoid this wobbling is to change a direction only if it is absolutely clear (beyond the measurement uncertainty) that this change will improve the robot's performance. The idea has indeed been successfully implemented in robotics [3,5].

The inertia phenomenon is behind the *asymmetric (libertarian) paternalism* idea, when, e.g., to encourage schoolkids to eat healthy food, we first restrict their menu to healthy choices, after which, when all the foods are introduced, they will be reluctant to switch [2,6]. In the talk, we explain how this phenomenon can be also used in education.

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Keywords: interval uncertainty; asymmetric paternalism; decision making

Solving Large Banded Systems of Linear Equations with Componentwise Small Error Bounds

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Linear systems with banded matrices and difference equations are closely related. Methods used to solve difference equations can be used to solve banded linear systems and vice versa. We present an algorithm based on QR factorizations providing appropriate coordinate systems – local to the computation of intermediate results – to fight against the wrapping effects of interval LU-factorization and interval forward/backward solving. The auxiliary matrices to be factorized by QR decomposition are of low dimension related to the bandwidth of the original system matrix. We present, in some detail, a C-XSC implementation of the algorithm. Numerical results and timings with systems up to several million unknowns are discussed. We also compare the accuracy of our results to the accuracy of methods using a lower bound on the smallest singular value.

Keywords: Banded interval linear systems, self-verifying numerical methods, C-XSC.

Interval Methods for Solving Underdetermined Nonlinear Equations Systems[1]

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The following problem is considered: enclose all solutions of the equations system $f(x) = 0$, where $x \in [\underline{x}, \overline{x}]$ and $f\colon \mathbb{R}^n \to \mathbb{R}^m$, $m < n$. Surprisingly, very little effort has been done to solve it, up to now. It is mentioned by some books (e.g. [3], [6]), but not considered in details. Also [2] investigates equations systems with non-square Jacobi matrix, but in a very specific context. Notably, a few papers consider a related problem: to find one solution of an under-determined system (see [7], [8]); it is a quite different problem, though; techniques for solving it are also different (e.g. they use preconditioning using a Moore-Penrose inverse, which would result in losing some solutions in our case).

The paper considers the branch-and-bound method and Newton operators adapted for under-determined systems. In this case the solutions form a manifold so they are (in general) not unique. Consequently, usual methods of verifying the uniqueness of a solution are not applicable, but we may modify them to verify that a box contains a segment of the solution manifold.

For the Newton operator, traditional approaches like interval Gauss-Seidel step or interval Gaussian elimination are not applicable directly (the matrix has no diagonal). It seems the Newton step computation should rather be considered as a constraint satisfaction problem. Narrowing operators may be obtained either from traditional linearization (e.g. [6]), from Kolev linearization [5] or the componentwise Newton step [1]. A few heuristics to choose the variable and the equation for narrowing are considered.

Theorems, describing some basic properties of considered methods, are proved, too. In particular, they imply that if for some equation and some variable double-sided improvement has been obtained, no more narrowing can be gained from this equation (before considering other ones). More specific propositions give conditions for checking if there is a segment of solution manifold in the box and for possibility of improving the upper or lower bound for a variable.

Other details are also briefly considered, like the possibility (and usability) of preconditioning for such systems or parallelization of the method.

Preliminary numerical results are presented.

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Keywords: underdetermined equations systems, interval Newton operators, componentwise Newton operator, constraint satisfaction

Accurate Solution of Triangular Linear System

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Compensated algorithms improve the accuracy of the computed solutions only using a unique computing precision, *e.g.* the IEEE-754 double precision. Previous results are related to summation and dot product [1] and to polynomial evaluation [2]. These compensated algorithms are proved to yield a solution as accurate as the original algorithm performed in twice the working precision and so provide an alternative to implementations with double-double arithmetic from [3]. In practice these compensated algorithms are measured to be at least twice faster than their double-double counterparts.

We consider the compensated solution of a triangular linear system $Tx = b$, where the matrix T and the vector b are floating-point entries of precision $\mathbf{u}$.

We exhibit that compensating the classic backward substitution algorithm is actually equivalent to one step of iterative refinement with a residual computed in extended precision. So a compensated algorithm for triangular systems only depends on the choice of the algorithm that computes the residual. We introduce two compensated algorithms: one uses error free transformations for the residual, the other uses the well known Dot2 algorithm from [1]. We prove an accuracy bound satisfied by the backward substitution algorithm with one step of iterative refinement when the residual is (at least) computed in twice the working precision. We derive that the accuracy of the compensated solutions $\overline{x}$ verifies the following bound,

$$\frac{\|\overline{x} - x\|_\infty}{\|x\|_\infty} \leq \mathbf{u} + K(T,x) \times \mathcal{O}(\mathbf{u}^2) + \mathcal{O}(\mathbf{u}^3).$$

The factor $K(T,x)$ is such that

$$\mathrm{cond}(T,x) \leq K(T,x) \leq \mathrm{cond}(T)\mathrm{cond}(T,x),$$

where $\mathrm{cond}(T)$ and $\mathrm{cond}(T,x)$ are the classic Skeel condition numbers. So we can not conclude that the compensated algorithms behave as the backward substitution implemented with double-double arithmetic. We discuss the proposed *a priori* bound compared to the one that applies to the backward substitution with double-double arithmetic. We present numerical experiments to exhibit that the actual accuracy of the compensated algorithms is similar to the double-double one. We measure that these accurate solutions of triangular linear systems are computed significantly

faster than with double-double arithmetic —as it is the case for previously known compensated algorithms [1,2].

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Applications of Constraints and Fuzzy Measures in Finance

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The aim of this paper is to address the following questions:

(1) How can we achieve a maximum return on investment in a portfolio for a given and pre-defined level of risk and

(2) What type of risk is necessary to achieve a given a pre-defined return on investment in a portfolio?

It is clear that to acquire wealth, some level of risk is necessary. Arbitrage ensures (at least in theory) that it is not possible to increase your assets, without some uncertainty associated with it. The higher the value of the expected return, the greater the degree of risk associated with the portfolio. We approach both problems from two different perspectives: as a constrained optimization problem and as a multi-criteria decision making problem.

The first approach seeks the optimal solution given a set of constraints, such as the required return, the maximum amount of money available to invest, and the non-negative amount of the investments, to name a few. The second approach addresses the same questions by constructing an aggregation operator to combine the impact of all criteria considered when choosing an optimal portfolio.

We present solutions to portfolio management from both perspectives with several twists of both approaches, together with their advantages and drawbacks. One common problem in modeling portfolio management, regardless of the solving method, is that the risk and the return are approximated based only on an expected behavior of the market, which is not known in advance. Thus, we face uncertainty in the level of risk each asset involves, as well as imprecision in the return that can be expected from any investment portfolio. To cope with these problems, we introduce intervals and represent risks and returns as ranges of values rather than single numbers. The resulting risk of a given portfolio is therefore given as an interval of values, from which we cannot clearly determine the optimal portfolio since comparing intervals is not as straightforward as comparing real numbers. Some strategies are presented to explain how to order intervals and therefore, to have a sound approach to address the problems presented initially.

Keywords: Investment portfolio, constraints, fuzzy measures, decision-making

Using Preference Constraints to Solve Multi-Criteria Decision Making Problems

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Many problems can be formulated in terms of decision making. Some decisions are relatively straightforward. However, other problems may require more strategizing such as decision pervaded by uncertainty (decision under uncertainty), or decision over multiple dimensions (multi-criteria decision making). The first problem faced with different criteria used to make the decisions is the domain of values each criterion can take. Some criteria take qualitative values while others take quantitative values that might be discrete or continuous. For example, when buying a car, we might consider its color, the safety rating, and the price. The color could be expressed using qualitative values (e.g. {red, black, grey}); the safety rating could be expressed using discrete integers representing the number of stars rating a car's safety (e.g. {1,2,3,4,5}); and the price could be expressed in terms of a continuous variable taking values within an interval (e.g. $[11000, 53000]$).

Furthermore, we have preferences within each criterion in terms of the values we would rather choose compared to other possible values of the criterion. However, only in miracle situations, an alternative that we can choose is characterized by the best value for each criterion. In most cases, we have to achieve some tradeoffs among criteria. On the other hand, we do not want to choose an alternative that is characterized by the worst values for each criterion. Thus, we need to narrow the search space from all possible values that criteria can take to a smaller space that contains the best choice (alternative) based on the preferences of an individual.

To solve this problem, we propose a method that is based on our belief that each individual is able to express the preference of a criterion over another criterion by means of how much of a criterion he/she would sacrifice in order to obtain higher value of the other criterion. For example, the individual knows how much more he/she is willing to pay for an increase in one star of safety rating. Further, we propose a method to utilize these individual's preferences in order to narrow the search space.

To accomplish the goal, we first map the domain of each criterion into an interval and consider the cross product of the intervals as the original scope of the solution. We use the preferences as constraints on the search space, and solve the constraints to narrow down the scope of the multi-criteria decision making problem.

A Digital Watermarking Method Using Interval Arithmetic

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We propose a new digital watermarking method using interval arithmetic. To the best of the author's knowledge, interval arithmetic has never been used in digital watermarking. This work is a first step toward a new application of interval arithmetic. Briefly stated, our method consists of wavelet transforms and interval arithmetic. By regarding interval expansion as useful information which computers produce automatically, we are applying interval arithmetic to the field of digital watermarking.

Experimental results demonstrate that the proposed method gives the better-quality watermarked image and has the robustness against some attacks.

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Keywords: interval arithmetic, digital watermarking, wavelet transform

Enclosing All Eigenvalues in Generalized Eigenvalue Problem

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In this presentation, we are concerned with the accuracy of computed eigenvalues λ in the generalized eigenvalue problem

$$Ax = \lambda Bx, \quad A, B \in \mathbb{C}^{n\times n},\ \lambda \in \mathbb{C},\ x \in \mathbb{C}^n, \tag{1}$$

where B is nonsingular. The problem (1) arises in many applications of scientific computations, e.g. stationary analysis of circuits, image processing, structure analysis and so forth.

There are several methods for calculating guaranteed error bounds for approximate eigenvalues and eigenvectors, e.g. [1-8]. The methods in [1,2,7,8] are applicable if A is Hermitian and B is Hermitian Positive definite. On the other hand, the methods in [4,5] are applicable even if A is not Hermitian and/or B is not Hermitian Positive definite. Especially in [5], methods are presented for computing enclosure of multiple eigenvalues and a basis for a corresponding invariant subspace. Note that the methods in [4,5] enclose *a few specified* eigenvalues and eigenvectors. In [6] it is shown how to compute an inclusion of an individual eigenvector to a multiple eigenvalue of geometric multiplicity one.

In this presentation, we present a theorem on enclosing *all* eigenvalues in (1). This theorem is applicable even if A is not Hermitian and/or B is not Hermitian Positive definite. Moreover we present theorems for accelerating the enclosure, which is based on a priori error estimation of floating-point arithmetic. Based on these theorems, we propose a fast method of enclosing *all* eigenvalues. The proposed method supplies an error bound ε such that $\lambda \in \bigcup_{i=1}^{n} \left\{ z \in \mathbb{C} \,\middle|\, |z - \tilde{\lambda}_i| \le \varepsilon \right\}$ for all λ, where $\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n$ denote approximate eigenvalues, in the case that all approximate eigenvalues and eigenvectors are given. Moreover the proposed method takes into account the presence of underflow in floating-point arithmetic.

From the results of numerical examples, we confirmed that the proposed method supplied error bounds of sufficient quality. We also confirmed that the computing time for the proposed method was comparable to that for calculating all approximate eigenvalues.

As an application of the proposed method, we also sketch an efficient method of enclosing all eigenvalues λ in polynomial eigenvalue problem

$$(\lambda^m A_m + \cdots + \lambda A_1 + A_0)x = 0, \quad A_0, \ldots, A_m \in \mathbb{C}^{n\times n},\ \lambda \in \mathbb{C},\ x \in \mathbb{C}^n, \tag{2}$$

where A_m is nonsingular. The problem (2) with $m = 2$ arises in, e.g. acoustic systems, electrical circuit simulation and structural mechanics.

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Keywords: Guaranteed Enclosure, Generalized Eigenvalue Problem, Non-Hermitian Case

Interval Finite Elements and Uncertainty in Engineering Analysis

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In recent years, there has been an increased interest in the modeling and analysis of engineered systems under uncertainties. The interest stems from the fact that numerous sources of uncertainty exist in reality and arise in the modeling and analysis process. Some of these uncertainties stem from factors that are inherently random (or aleatory). Others arise from the lack of knowledge (or epistemic).

These facts make us to believe that uncertainty is unavoidable in engineering systems. Solid and structural mechanics entails uncertainties in material, geometry and load parameters.

Latest scientific and engineering advances have started to recognize the need for defining multiple types of uncertainty. Probabilistic approach is the traditional approach that requires sufficient information to validate the probabilistic model. Probabilistic modeling cannot handle situations with incomplete or little information on which to evaluate a probability, or when that information is nonspecific, ambiguous, or conflicting. Many interval-based uncertainty models have been developed to treat such situations. These generalized models include fuzzy sets and possibility theory, Dempster-Shafer theory of evidence, random set theory, probability bounds, imprecise probabilities, convex model, and others.

This talk presents an overview of interval approaches for the treatment of uncertainty for structural mechanics problems. Uncertain parameters are introduced in the form of unknown but bounded quantities (intervals). Interval analysis is applied to the Finite Element Method FEM) to analyze the system response due to uncertain stiffness and loading.

Overestimation in interval analysis represents the main challenge in obtaining sharp enclosures to the system response. The main source of such overestimation is the treatment of multiple appearances of the same variable as if they were independent; in fact, whatever value a variable assumes in one instance, it must be the same in the other. A number of methods have been developed to handle this overestimation such as the Element-By-Element (EBE) technique [1], [2], [3]. Where element matrices are formulated based on the physics of materials, and the Lagrange multiplier method is applied to impose the necessary constraints for compatibility and equilibrium. Based on the developed formulation, the bounds on the system's displacements and element forces are obtained simultaneously and have the same level of accuracy. Very sharp enclosures for the exact system responses are obtained. A number of numerical examples are introduced, and scalability is illustrated.

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Keywords: Interval, Finite Elements, Uncertainty, Engineering Mechanics

Exact Hull of Linear Interval Equations with Matricies Arising from Engineering Applications

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In an earlier paper by the authors (Muhanna et al. 2001), it was observed that for a class of problems known by structural engineers as statically determinate, sharp interval bounds were obtained for a parametric system of equations generated by an interval extension to matrix structural analysis. While a statically determinate problem can be readily identified by an engineer based on the initial description of the problem, the identification of a statically determinate problem from the system of algebraic equations resulting from a stiffness structural analysis was not known.

In this paper, we present a definition of the property of the structural stiffness matrix that is a generalization for the concept of a statically determinate problem.

Such a structural stiffness matrix has the following properties:

1) The non-singular interval matrix is the sum of non-interval component matrices that are multiplied by interval parameters.

2) Each component matrix is symmetric and non-negative definite.

3) The overall matrix sum is positive definite.

4) Setting any one of the interval multiplicative parameters to zero results in the overall matrix becoming singular.

From this definition, one can show that the sharp interval hull of the solution of such a system of simultaneous equations can be found in polynomial time. An algorithm for calculating the interval hull of the solution for this class is presented. An algorithm for the eigenvalue decomposition of this class of matrices is also given. Example problems from engineering analysis are presented to illustrate the application of the algorithms. Results are compared to more general interval finite element solutions that do not utilize the properties of this class matrices. Comparisons include the width of the interval solutions as well as the computational effort required. Such matrices present an interesting class of interval matrices that arise out of engineering problems.

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Keywords: Interval systems, Finite Elements, Determinate Structures, Exact Hull

A Differential Inequalities method for Verified Solution of IVPs for ODEs using Linear Programming for the Search of Tight Bounds

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In his survey [1], Nedialkov stated that "Although high-order Taylor series may be reasonably efficient for mildly stiff ODEs, we do not have an interval method suitable for stiff ODEs." This paper is an attempt to find such a method, based on differential inequalities. Assume we have an IVP for ODE $\dot{y}(t) = f(y(t), t)$, $y(0) \in [y_0]$, $y(t) \in \mathbb{R}^n$ and we want to compute the bounds of $y(h)$. Assume also that the right-hand side function $f(y,t)$ is bounded by lower and upper bounds $\underline{f}(y,t) \le f(y,t) \le \overline{f}(y,t)$. As in [2], we use Müller's theorem from the theory of differential inequalities. We need to guess $2n$ functions $\underline{y}_i(t)$ and $\overline{y}_i(t)$ such that

$$[y_{0i}] \subset [\underline{y}_i(0), \overline{y}_i(0)] \tag{1}$$

$$\dot{\underline{y}}_i(t) \le \underline{f}_i(y,t) \qquad \text{if } y \in [\underline{y}(t), \overline{y}(t)] \text{ and } y_i = \underline{y}_i(t) \tag{2}$$

$$\dot{\overline{y}}_i(t) \ge \overline{f}_i(y,t) \qquad \text{if } y \in [\underline{y}(t), \overline{y}(t)] \text{ and } y_i = \overline{y}_i(t) \tag{3}$$

for all $t \in [0,h]$. Then $y_i(h) \in [\underline{y}_i(h), \overline{y}_i(h)]$. The conditions (1)-(3) can be verified for given functions $\underline{y}(t)$ and $\overline{y}(t)$ by interval computation [3].

For a test IVP $\dot{y}(t) = \lambda y$, $y(0) \in [0,1]$ ($\lambda < 0$) we guess a pair of linear functions $[\underline{y}(t), \overline{y}(t)] = \left[0, \dfrac{1+\lambda(t-h)}{1-\lambda h}\right]$ which satisfy (1)-(3). The bound of $y(h)$ is $\left[0, \dfrac{1}{1-\lambda h}\right]$. Its width decays to zero when $h \to \infty$, demonstrating suitability of the method for stiff ODEs. However, the problem is to find the bound functions in a regular way.

If we restrict $\underline{y}$ and $\overline{y}$ by polynomials of degree r, the search space will have dimension $2n(r+1)$. Consider a few optimization problems in this search space with common constraints (1)-(3) and with targets like $\underline{y}_i(h) \to \max$, $\overline{y}_i(h) \to \min$, $\overline{y}_i(h) - \underline{y}_i(h) \to \min$. Each problem returns a bounding box for $y(h)$. The intersection of these boxes also bounds $y(h)$.

If $\underline{f}(y,t)$ is concave function of y and $\overline{f}(y,t)$ is convex function of y for any $t \in [0,h]$, then each optimization problem becomes a convex problem. A local minimum of a convex problem is a global minimum [4]. Though the bounds maybe high-order polynomials, the optimization algorithm requires only low-order derivatives of $f(y,t)$. This is good for applications with an empirical region-wise definition $f(y,t)$.

Differential inequalities can be used also to bound the deviation of the true solution from the approximate solution $\hat{y}$ found by other validated or non-validated methods. In this case we can

bound the function by its linear approximation near the approximate solution $f(y,t) \in f^I(\hat{y}(t),t) + [J(t)](y - \hat{y}(t))$. When $[f(y,t)] = [J]y + [b(t)]$, $\underline{b}(t)$ and $\overline{b}(t)$ are linear and $r = 1$, the optimization problem becomes a linear programming problem. The initial solution basis for the LP algorithm at the timestep can be borrowed from the previous timestep to have fewer iterations.

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Keywords: Validated method, Differential Inequalities, Convex Programming, Linear Programming

Validated Computations for Elliptic Systems of Fitzhugh-Nagumo Type

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We consider the reaction-diffusion system:

$$\begin{cases} \dfrac{\partial u}{\partial t} = D_u \triangle u + f(u,v) & \text{in } \Omega, \\ \dfrac{\partial v}{\partial t} = D_v \triangle v + g(u,v) & \text{in } \Omega, \end{cases} \tag{1}$$

where Ω is a bounded convex domain in $\mathbf{R}^n$ $(n = 1, 2, 3)$ with piecewise smooth boundary $\partial\Omega$, and the parameters $D_u,\ D_v$ are positive constants. Especially we treat systems of FitzHugh-Nagumo type, i.e. we assume that f and g have the following form:

$$\begin{cases} f(u,v) = u(1-u)(b+u) - \delta v & (b, \delta \in \mathbf{R}), \\ g(u,v) = \epsilon(u - \gamma v) & (\epsilon, \gamma \in \mathbf{R}). \end{cases} \tag{2}$$

Our aim is to enclose the steady-state solutions of (1) with Dirichlet or Neumann boundary conditions. We present a method for enclosing the steady-state solutions based on computer assisted means. Some numerical examples will be shown.

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Keywords: Validated Computation, Reaction-Diffusion Equations, Fixed Point Theorem, Error Estimates

An Interval Newton Method based on the Bernstein Form for Bounding the Zeros of Polynomial Systems

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Interval Newton methods are widely used to find reliable enclosures for the zeros of systems of polynomial equations in a given search region. At each iteration, the interval Newton operator needs not only the evaluation of the polynomial system at a particular point, but also needs the derivative enclosures over the current search box [1]. These evaluations can be time consuming, especially if the evaluation of derivatives is done via normal interval arithmetic or automatic differentiation. Further, the resulting derivative enclosures can be quite pessimistic, necessitating a large number of Newton iterations. To overcome these difficulties, we propose an alternative approach based on Bernstein polynomial coefficients [2] to compute the value of the Newton operator. The new so-called Bernstein Newton method does not require the function evaluation at any point, while the computation of the derivative enclosures becomes very simple and much sharper. The increase in sharpness is due to the fact that the range enclosure obtained from Bernstein coefficients is often much sharper than the range enclosure obtained with many interval forms [3]. We compare the performance of the proposed Bernstein Newton method with that of the Interval Newton method on two numerical examples. The results show that the proposed method takes less iterations and time than the interval Newton method.

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Keywords: Bernstein polynomials, Interval Analysis, Interval-Newton method, Polynomial systems, Root finding.

The Extrapolated Taylor Model

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The Taylor model [1] is one of the inclusion functions available to compute the range enclosures. It computes a high order polynomial approximation to a multivariate Taylor expansion, with a remainder term that rigorously bound the approximation error. Sharper bounds on the enclosures computed using the Taylor model can be obtained either by successively partitioning the domain using suitable subdivision factors, or by increasing the convergence rate of the Taylor model using higher order Taylor models. However, higher order Taylor forms require higher degrees of the polynomial part, which in turn require more computational effort and more memory. This is the major drawback of increasing the order of Taylor models for obtaining range enclosures with higher order convergence rates. In this paper, we attempt to overcome these drawbacks by using a lower order Taylor model, and then using extrapolation to accelerate the convergence process of the sequences generated with the lower order Taylor model. The effectiveness of all the proposed algorithms is tested on various multivariate examples and compared with the conventional methods. The test results show that the proposed extrapolation-based methods offer considerable speed improvements over the conventional methods

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Keywords: Asymptotic Expansion, Extrapolation Methods, Richardson Extrapolation, Interval Analysis, Taylor model.

On the Blunting Method in Verified Integration of ODEs

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Interval methods for ODEs often face two obstacles in practical computations: the dependency problem and the wrapping effect. The dependency problem can be characterized as the failure of interval arithmetic in recognizing several instances of the same variable in a given expression. The wrapping effect introduces overestimation when some set in $\mathbb{R}^n$ describing an intermediate result of a calculation is enclosed into an interval box in n dimensions. Taylor model methods, which have been developed by Berz and his group, have recently attracted attention. By combining interval arithmetic with symbolic calculations, these methods suffer far less from the dependency problem than traditional interval methods for ODEs. By allowing nonconvex enclosure sets for the flow of a given initial value problem, Taylor model methods have also a high potential for suppressing the wrapping effect.

Makino and Berz advocate the so-called blunting method. In this talk, we analyze the blunting method (as an interval method) for a linear model ODE. We compare its convergence behavior with that of the well-known QR interval method.

We consider a Taylor series method with constant stepsize h and order p on the test problem

$$y' = Ay, \quad y(0) = y_0 \in \boldsymbol{y}_0,$$

where $y \in \mathbb{R}^n$, $A \in \mathbb{R}^{n\times n}$, $n \geq 2$, and $\boldsymbol{y}_0$ is a given interval vector, accounting for uncertainty in initial conditions.

It can be shown that the amount of overestimation of the flow of the initial set depends on the spectral radius of a certain matrix. We consider the case that

$$T := \sum_{i=0}^{p-1} \frac{(hA)^i}{i!}$$

has eigenvalues of distinct magnitudes. Then the spectral radii of the matrices that describe the excess propagation in the QR method and in the blunting method, respectively, have the same limits, so that the excess propagation in both methods should be similar. This theoretical result is confirmed by numerical examples.

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Solving and Certifying the Solution of a Linear System

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We propose an approach to solve a linear system and at the same time certify the calculated solution. To certify this solution, we compute an enclosure of the error: we switch from floating-point arithmetic to interval arithmetic to solve the residual system and this yields a guaranteed enclosure of the error on the exact result.

The use of the residual is classical in iterative refinement methods. We have adapted the iterative refinement for the computation of an enclosure of the error. These two building blocks, i.e., the floating-point solution of a linear system and the iterative refinement of the error bounds using interval arithmetic, are combined to produce a more accurate solution along with a tight enclosure of the error. Furthermore, the error bound yields the number of correct digits of the approximate solution.

Another question naturally arises: it is well known that the accuracy of the iteratively refined solution relies for a large part on the computing precision used for the residual calculation. Classically, the computing precision is doubled for the residual calculation. Our algorithms are implemented using the MPFR library, that offers arbitrary precision floating-point arithmetic, and MPFI for the interval counterpart. These libraries enable us to tune the computing precision of each step, and we also study the influence of the computing precision for the residual calculation on the solution accuracy.

Let's now enter into the details of our implementation. For the floating-point part, namely the solution of the linear system, the chosen method is simply the LU factorization of the matrix of the system, followed by forward and backward substitutions. We re-use this LU factorization to precondition the linear system, for the interval part. In the interval part, the residual is computed using interval arithmetic. Then a small constant number of iterations of the Gauss-Seidel method are performed; this yields an enclosure of the error. The approximate solution can then be updated: the center of the error interval is used as a corrective term and is added to the solution. The interval part can be iterated, with increasing computing precision. Experiments illustrate the gain in accuracy on the solution and on the error, related to the employed computing precision.

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Keywords: linear system solving, interval arithmetic, iterative refinement, computing precision, accuracy, certification.

Verified Numerical Computation of Matrix Determinant

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In this talk, a numerical verification method for computing the determinant $\det(A)$ for a real $n \times n$ matrix A is proposed using matrix decompositions.

Let us assume that some computed LU factors of A are given such that $PA \approx LU$, where P is a permutation matrix following partial pivoting during the LU factorization, L is a unit lower triangular matrix, and U is an upper triangular matrix, respectively. Then a well-known method [2, (14.34)] to compute an approximation of the determinant is to use products of diagonal elements of U:

$$\det(A) \approx \det(P^T LU) = \det(P) \det(U).$$

On the other hand, some verification methods for the matrix determinant (cf. e.g. [1,3]) have been proposed. For example, Rump [3] has presented an efficient verification method, which is based on the following fact: Let X_L and X_U be approximate inverses of L and U, respectively. Let $B := X_L PAX_U$. Then

$$\det(B) = \det(P) \det(A) \det(X_U)$$

and

$$\det(A) = \frac{\det(P) \det(B)}{\det(X_U)},$$

because $\det(X_L) = 1$. Here, it can be expected that B is nearly the identity matrix I, which is almost diagonal, and $\det(B) \approx 1$. So, Gershgorin's circle theorem gives (an enclosure of) the product of all eigenvalues of B, which implies an enclosure of $\det(B)$. It turns out that an enclosure of $\det(A)$ can also be computed.

Let us present an another approach to verify the matrix determinant. If A is nonsingular, then there exists E such that

$$PA(I + E) = LU.$$

Then $E = A^{-1} P^T LU - I$.

$$\det(A) = \frac{\det(P) \det(U)}{\det(I + E)}.$$

If $\|E\| \ll 1$, then $I + E$ is almost the identity matrix and $\det(I + E) \approx 1$. Again using Gershgorin's circle theorem, an enclosure of the product of all eigenvalues of $I + E$ can be computed, which implies an enclosure of $\det(I + E)$, and so can an enclosure of $\det(A)$.

We will also present several verification methods for the matrix determinant. Detailed algorithms and numerical results will be presented.

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Keywords: verified numerical computation, matrix determinant, floating-point filter, rounding error analysis

Accurate and Fast Sum of Floating Point Numbers and Applications to Verification Algorithms

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Let $\mathbb{F}$ be a set of floating point numbers satisfying suitable conditions. For instance, in this talk the system satisfying IEEE 754 standard is con- sidered. With S. M. Rump and T. Ogita, the author [1], [2] has developed a method of calculating $\mathbf{res} \in \mathbb{F}$ satisfying

$$\frac{|\mathbf{res} - \sum p_i|}{|\sum p_i|} \leq c \cdot \mathbf{u}_{\mathrm{out}}$$

independent of the condition number of the sum of $p_i \in \mathbb{F}$, where $\mathbf{u}_{\mathrm{out}}$ is a machine epsilon. The proposed algorithm has the following characteristics:

- only the sum and product of the floating point arithmetic are used,
- no if statements nor branches

which imply

- no need of special hardware,
- fast.

For this purpose, the authors have proposed the concept of the error free transformation (EFT, for short). Two typical examples of EFT are Knuth's two-sum algorithm and Veltcamp and Dekker's two-product algorithm. The authors have developed a new type of EFT which split a floating point number into two floating point numbers with desired properties. Using this, they have proposed a fast accurate sum algorithm of floating point numbers with desired properties.

A first part of this talk will explain the algorithm. It will be shown that the algorithm always gives accurate result independent of condition numbers of the problems. Further, it will also be clarified that a real speed of calculating sum is very fast.

Then, in the second part of the talk, the following applications of the accurate sum will be discussed:

- application to Rump's algorithm of inverting arbitrary ill-conditioned rectangular matrices,
- iterative refinement algorithm for linear equations,
- computational geometry algorithms which never fail,

- other applications.

As a result, it will be clarified, for instance, that a fast adaptive algorithm, which uses only working precision floating point arithmetic, can now be constructed which always gives an approximate solution $\tilde{x}$ for

$$Ax = b; \quad (A \in \mathbb{F}^{n \times n}, b \in \mathbb{F}^n)$$

satisfying

$$\frac{\|\tilde{x} - A^{-1}b\|_\infty}{\|A^{-1}b\|_\infty} \leq c \cdot \mathbf{u}_{\text{out}}$$

independent of its condition number provided that A is regular.

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Keywords: Error-free transformation, Accurate sum, Ill-conditioned matrices

Interval Computations are Also Useful for Statistical Estimates

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In many real-life situations, we are interested in the value of a physical quantity y that is difficult or impossible to measure directly. Since we cannot measure y directly, a natural idea is to measure y indirectly. Specifically, we find some easier-to-measure quantities $x_1, \ldots, x_i, \ldots, x_n$ which are related to y by a known relation $y = f(x_1, \ldots, x_i, \ldots, x_n)$; this relation may be a simple functional transformation, or complex algorithm. Then, to estimate y, we first measure the values of the quantities $x_1, \ldots, x_i, \ldots, x_n$, and then we use the results $\widetilde{x}_1, \ldots, \widetilde{x}_i, \ldots, \widetilde{x}_n$ of these measurements to compute an estimate $\widetilde{y}$ for y as $\widetilde{y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_i, \ldots, \widetilde{x}_n)$. Due to the measurement errors $\Delta x_i \stackrel{\text{def}}{=} \widetilde{x}_i - x_i \neq 0$, the estimate $\widetilde{y}$ is, in general, different from the desired actual value y. How can we estimate the resulting error $\Delta y \stackrel{\text{def}}{=} \widetilde{y} - y$?

In the traditional engineering approach, we usually assume that all the measurement errors Δx_i are independent and normally distributed, with 0 mean and known standard deviations σ_i. In practice, however, we are not sure about the independence and/or about 0 mean. In many cases, the only information that we have is the upper bound Δ_i on the measurement error: $|\Delta x_i| \leq \Delta_i$. In this case, our only information about each actual value x_i is that x_i belongs to the interval $\mathbf{x}_i = [\widetilde{x}_i - \Delta_i, \widetilde{x}_i + \Delta_i]$, and the range $\mathbf{y} = \{f(x_1, \ldots, x_n) \,|\, x_i \in \mathbf{x}_i\}$ of y can be estimated by using the traditional interval computations technique.

The traditional statistical approach and interval computations form two extremes: in the first case, we have a full information about all the probabilities of the measurement errors Δx_i, while in the interval case, we know nothing about the probabilities. In reality, we usually have partial information about the probabilities: e.g., we often know that the measurement errors are independent, and that the distributions are (almost) Gaussian: Gaussian restricted to the given intervals. How can we use this additional knowledge in estimating Δy?

It turns out that even with this additional information, we get the same set $\mathbf{y}$ of all possible values of y as for interval computations, and for each subinterval from this interval, the probability for y to be in this subinterval can take any value between 0 and 1. Thus, even in this seemingly statistical situation, in which we have a large amount of knowledge about probabilities, we have to use interval computations.

Keywords: interval computations, statistical estimates

Tight Inclusion of Matrix Multiplication and Its Portable Implementation

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This talk is concerned with an accurate interval arithmetic. In particular, we provide a tight inclusion of matrix multiplication, which avoids overestimation of a radius of the interval arithmetic. Let A and B be a floating-point m-by-n matrix and a floating-point n-by-p matrix respectively. To compute an inclusion of AB, the rounding mode controlled computation is widely used, in which floating point matrix multiplication is computed twice to obtain an interval result by switching rounding upward and downward respectively so that it requires $4mnp$ flops (flops means floating-point operations). A fast interval arithmetic for matrix multiplication can be developed by an a priori error analysis, whose computational cost is $2mnp$ flops. Our purpose is to develop a method which is more robust than these two methods.

Recently, accurate summation algorithms were developed by Rump-Ogita-Oishi [2,3]. One of the key techniques in their methods is a new error-free splitting algorithm. These methods avoid using a sorting for input data, branch in each of the main loop and direct access for mantissa or exponent bit, which slows the computational speed. Therefore, their methods are fast in terms of measured computing time.

To adopt this strategy to the matrix multiplication, we can split A and B into sum of matrices $\sum_{i=1}^{e} A^{(i)}$ and $\sum_{j=1}^{f} B^{(j)}$ for some integers e, f, respectively. After these splittings, we compute the matrix products $A^{(i)}B^{(j)}$ $(1 \leq i \leq e, 1 \leq j \leq f)$. We notice that a part of matrix products can be computed without rounding errors. Combining a fast inclusion technique [1] with this approach, the tight inclusion of matrix multiplication involves $6mnp$ flops when $e = f = 2$.

There is a significant advantage in the proposed method; we can mainly use the level 3 BLAS (Basic Linear Algebra Subprograms) operation. Therefore, a specific multi-precision library is not necessary to obtain a tight inclusion of AB. BLAS is optimized to each architecture so that the optimized BLAS achieves near peak performance.

The switch of rounding mode is not supported on some computer environments, for example, FORTRAN 77 and Java. In these environments, the interval arithmetic for matrix multiplication must be computed by using only rounding to nearest mode. However it is easy to adapt our algorithm to such computer environments by changing our algorithm slightly.

At the end of the talk, some numerical examples are presented for illustrating the effectiveness of the proposed method.

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Keywords: Interval Arithmetic, Accurate Computing.

Gait Analysis Using Optimization and Constraint Programming Techniques

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Many neurological diseases, such as cerebral palsy in children, strokes or Parkinson's disease, can cause abnormal changes in gait or "gait disorders" and significantly affect the ability of patients to walk without assistance. Intensive rehabilitation therapy is usually the key for patients to improve their walking ability. However, therapy is usually long and relies on human experts to perform it: it involves a lot of repetition of exercises guided by therapists. As a result, it is not as efficient as one would expect and it is very costly. The key to improve rehabilitation is to automate the diagnosis of gait pathologies and as well as the therapy.

Automatically diagnosing gait pathologies requires to be able to assess gait. Nowadays, gait is assessed through observation and/or computer-based analysis of some characteristics; e.g., the angle between the shinbone and the femur, the height of the ankle (using markers placed on the patient's joints: typically ankle, knee, hip). Current diagnosis techniques are based on observations [3]; current research on automating the gait diagnosis makes use of video and data recordings. Current research work is mostly oriented towards the use of fuzzy logic [1,2] or neural networks [5,6], in order to identify features that will help differentiate between healthy and unhealthy gaits. Since it is also expected that diagnosis will involve comparing observed gait to known healthy gaits, current research is also concerned with being able to recognize scaling and shifting [4], so that comparison can be performed properly. However, although important, the problem of inconsistencies in the gait cycles of a same patient (e.g., patients walking faster, slower, patients having a very distorted gait) has not been addressed yet, and neither the need for determining models (of both healthy and unhealthy patients).

In this work, we focus on the diagnosis part of the problem. Our work makes use of optimization and constraint programming techniques, aiming at extracting characteristics (models) and at being independent of inconsistencies in the cycles / patients (e.g., height, weight, age) / speed. In particular, we propose a new technique to automatically detect gait cycles, and to determine whether or not a gait is unhealthy.

The work we describe in this abstract was performed on data recorded from healthy patients, and obtained from markers placed on their ankle, knee, and hip joints. We developed a simple filtering algorithm that takes into account online significant points among the recorded data, and that allows to exhibit a pattern of a normal gait. From the result of this algorithm, we were also able to isolate cycles and correlate them between data from different markers, in order to validate our patterns. The patterns were then used to define constraint solving problems: this step allows us to check if a gait is not healthy, i.e., does not match the expected pattern.

The novelty of this work for gait analysis lies on the fact that we are interested only in patterns, which leads us to a qualitative assessment of the gait, and not so much in a quantitative assessment that, in our opinion, relies too much on the data being perfect (no inconsistency).

Preliminary results show the promise of our work, and the developed tool can be extended to support the detection of more inconsistencies in the recordings than the ones experimented and reported in this article.

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Keywords: gait analysis, optimization, patterns, constraint programming.

From Gauging Accuracy of Quantity Estimates to Gauging Accuracy and Resolution of Field Measurements: Geophysical Case Study

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Most practical applications of interval computations deal with situations in which we process the measured values of the physical quantities $x_1, \ldots, x_n$ to estimate the value of a related difficult-to-measure y which is related to x_i by a known dependence $y = f(x_1, \ldots, x_n)$. Since measurements are never absolutely accurate, the measurement results $\widetilde{x}_i$ are, in general, different from the actual (unknown) values x_i of the measured quantities. Because of this, the result $\widetilde{y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_n)$ of data processing is, in general, different from the actual (unknown) value $y = f(x_1, \ldots, x_n)$. In practice, we often only know the upper bound Δ_i on the measurement errors $\Delta x_i \stackrel{\text{def}}{=} \widetilde{x}_i - x_i$: $|\Delta x_i| \le \Delta_i$. In this case, the only information that we have about the actual values x_i is that $x_i \in \mathbf{x}_i \stackrel{\text{def}}{=} [\widetilde{x}_i - \Delta_i, \widetilde{x}_i + \Delta_i]$. Interval computations can then be used to find the corresponding range $\mathbf{y} = \{f(x_1, \ldots, x_n) : x_i \in \mathbf{x}_i\}$ of the desired quantity y; see, e.g., [1].

In practice, the situation is often more complex: the values that we measure are values $v(t)$ of a certain dynamic quantity v at a certain moment of time t or, more generally, the values $v(x,t)$ of a certain physical field v at a certain location x and at a certain moment of time t. For example, in geophysics, we are interested in the values of the density at different locations and at different depth. For such measurements, not only we get the measured value $\widetilde{v} \approx v$ with some inaccuracy, but also the location x is not exactly known; moreover, the sensor picks up the "averaged" value of v at locations close to the approximately known location $\widetilde{x}$. In other words, in addition to inaccuracy $\widetilde{v} \neq v$, we also have a finite *resolution* $\widetilde{x} \neq x$. How can we describe the relation between these measurement results and the actual field values? How can we process such generalized interval data?

The answers to these questions clearly depend on what we know about the resolution.

In some cases, we know how the measured values $\widetilde{v}_i$ are related to $v(x)$, i.e., we know the weights $w_i(x)$ in $\widetilde{v}_i \approx \int w_i(x) \cdot v(x)\, dx$. In this case, all our information about $v(x)$ is contained in the set of values $\widetilde{v}_i$. In [4-6], we describe how to process such data.

In other cases – similarly to the standard interval setting – we only know the upper bound Δ_x on the location error $\widetilde{x} - x$. In this case, every measured pair $(\widetilde{v}_i, \widetilde{x}_i)$ must be (Δ, Δ_x)-close to some value $(v(x), x)$. This closeness can be naturally described in terms of an (asymmetric) Hausdorff distance $d(\widetilde{V}, V)$ between the set of measurement pairs $\widetilde{V}$ and the graph V of the field $v(x)$; this approach is similar to the one described in [1].

Yet another case is when we do not even know Δ_x; it happened, e.g., when we solve the seismic inverse problem to find the velocity distribution. In this case, a natural heuristic idea is to add a perturbation of size Δ_0 (e.g., sinusoidal) to the reconstructed field $\widetilde{v}(x)$, simulate the new measurement results, apply the same algorithm to the simulated results, and reconstruct the new field $\widetilde{v}_{\rm new}(x)$. If the perturbations are not visible in $\widetilde{v}_{\rm new}(x) - \widetilde{v}(x)$, this means that details of size Δ_0 cannot be reconstructed and so, the actual resolution is $\Delta_x > \Delta_0$. This approach was partially described in [2,7]. In this talk, we elaborate on it, and derive the optimal perturbations shape.

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Numerical Solution of the Problem of Large Forest Fires Initiation

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The paper suggested in the context of the general mathematical model of forest fires gives a new mathematical setting and method of numerical solution of a problem of a large forest fire initiation. Mathematical model of forest fire was based on an analysis of known experimental data and using concept and methods from reactive media mechanics. The forest and combustion products are considered as a homogeneous two temperatures, reacting, non-deformed medium. Temperatures of condensed and gaseous phases are separated out. The first includes a dry organic substance, moisture (water in the liquid-drop state), condensed pyrolysis and combustion products (coke, ash) and mineral part of forest fuels. In the gaseous phase we separate out only the components necessary to describe reactions of combustion (oxygen, combustible products of pyrolysis of forest fuels and the rest inert components). The solid phase constituting forest fuels has no intrinsic velocity, and its volumetric fractions, as compared to the gaseous phase, can be neglected in appropriate equations because a volume unit of wood. It is considered that

1) the flow has a developed turbulent nature, molecular transfer being neglected,

2) gaseous phase density doesn't depend on the pressure because of the low velocities of the flow in comparison with the velocity of the sound,

3) forest canopy is supposed to be non-deformed porous medium. The research is done by means of mathematical modeling of physical processes.

It is based on numerical solution of Reynolds equations for chemical components and equations of energy conservation for gaseous and condensed (for canopy) phases [2]. To describe the transfer of energy by radiation we use a diffusion approximation. To obtain discrete analogies a method of control volume of S.V.Patankar is used. Calculation method and program have been check. The boundary-value problem is solved numerically using the method of splitting according to physical processes. In the first stage, the hydrodynamic pattern of flow and distribution of scalar functions are calculated. The system of ordinary differential equations of chemical kinetics obtained as a result of splitting is then integrated. A discrete analog for equations is obtained by means of the control volume method. The accuracy of the program is checked by the method of inserted analytical solutions. Analytical expressions for the unknown functions are substituted in the system of differential equations and the closure of the equations are calculated. This is then treated as the source in each equation. Next, with the aid of the algorithm described above, the values of the functions are inferred with an accuracy of not less than 1%. The effects of the dimensions of the control volumes on the solution are studied by diminishing them. The time interval is selected automatically. As a result of mathematical modeling the fields of temperatures, mass

concentrations of components of gaseous phase, volume fractions of components of solid phase, as well as vectorial fields of velocity at different instants of time. It allows to investigate dynamics of forest fire initiation under influence of various external conditions.

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Keywords: resolution, accuracy, inverse problem, interval uncertainty

Computational Aspects of the Implementation of Disk Inversions

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Complex circular interval arithmetic, established by Gargantini and Henrici [1] in 1972, is convenient for bounding complex-valued solutions of equations or results of calculations involving complex variables. In this way, an automatic control of upper error bounds on approximate solutions or results is provided. In this paper we are concerned with the application of two kinds of disk inversions in the realization of simultaneous methods for the inclusion of complex zeros of polynomials.

In practice, we deal with two kinds of disk inversions:

$$\{c;r\}^{-1}=\Big\{\frac{\bar{c}}{|c|^2-r^2};\frac{r}{|c|^2-r^2}\Big\}=\{1/z:z\in\{c;r\}\ \ (0\notin\{c;r\})$$

(exact inversion) and

$$\{c;r\}^{I_c}=\Big\{\frac{1}{c};\frac{r}{|c|(|c|-r)}\Big\}\supset\{c;r\}^{-1}\ \ (0\notin\{c;r\})$$

(centered inversion). The implementation of iterative methods for the simultaneous inclusion of polynomial zeros in circular complex interval arithmetic is carried out for more than three decades by using the exact inversion of disks. Based on theoretical analysis and numerical examples, we show that the centered inversion leads to smaller inclusion disks. This surprising result is the consequence of better convergence of the midpoints of produced disks when the centered inversion is employed. The behavior of several inclusion methods with the centered and exact inversion is illustrated on numerical examples.

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Keywords: Circular complex arithmetic, polynomial zeros, inclusion disks

Diametrical Circular Form of Elementary Functions and Its Applications

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Information about the range of a function f is of great interest in the field of numerical and functional analysis, differential equations, linear algebra, approximation and optimization theory. The objective of this communication is to present a numerical tool for finding the smallest possible inclusion disk $F(Z)$ that entirely contains the exact range $f(Z)$ of a complex function f over a disk Z, that is, $F(Z) \supseteq f(Z) = \{f(z) | \, z \in Z\}$.

The best enclosing circular approximation to the range $f(Z)$ is, obviously, a disk with the diameter equal to the diameter D of the range $f(Z)$ if this disk completely contains $f(Z)$. Such a disk is called the *diametrical disk* and it is unique. The determination of the diametrical disk $I_d(f(Z)) := \{w; D/2\}$ centered at w for a given range $f(Z)$ leads to the two problems which are often difficult: 1) finding the diameter of the range $f(Z)$, and 2) checking the inclusion $f(Z) \subseteq \{w; D/2\}$ (see [1]). We give a list of diametrical disks form for elementary complex functions such as $\log z$, $\tan^{-1} z$, $\cot^{-1} z$, $\tanh^{-1} z$, $\coth^{-1} z$, e^z, z^n, $z^{1/k}$ over a given disk Z.

Although non-diametrical disks (such as circular centered form) most frequently have advantages in solving some problems because of their convenient properties (e.g., inclusion isotonicity), the use of diametrical disks is especially significant in various calculations in computational complex analysis (inclusive calculus of residues, numerical integration with uncertain data, etc.) and optimization theory where very sharp estimates are required. We illustrate the application of diametrical circular form in several examples. We emphasize that the design of a library of elementary complex functions f over a given disk Z in the diametrical form $I_d(f(Z))$, together with minimal circular arithmetic, is of interest in practical applications.

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Higher Order Methods for the Inclusion of Multiple Zeros of Polynomials

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Iterative methods for the simultaneous determination of complex zeros of a given polynomial, implemented in complex interval arithmetic, are very efficient device to error estimates for a given set of approximate zeros. This kind of self-verified methods possesses very important inclusion property consisting of the enclosure of the sought zeros in each iteration. The objective of this paper is to continue the research concerned with fast iterative methods for the simultaneous inclusion of polynomial zeros, which can be regarded as interval versions of Halley-like iterative method presented in [1] and [2]. Starting from suitable fixed point relation, we derive higher order iterative methods for the simultaneous inclusion of polynomial multiple zeros in circular complex interval arithmetic. Each of resulting disks contain one and only one zero in every iteration. This convenient inclusion property, together with very fast convergence, ranks these methods among the most powerful iterative methods for the inclusion of polynomial zeros. Using the concept of the R-order of convergence of mutually dependent sequences, we present the convergence analysis of the total-step and the single-step methods with Schröder's and Halley's corrections under computationally verifiable initial conditions. The proposed self-verified methods possess a great computational efficiency since the acceleration of the convergence rate from four to five and six is achieved without additional calculations. To demonstrate convergence behavior of the presented methods, two numerical examples are given.

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Uncertainty Processing in Cyberinsfrastructure, with Applications to Geosciences and to Environmental Science

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In the past, communications between computers were several orders of magnitude slower than computations. As a result, traditionally, data processing has been performed on a single computer. This computer may have been a multi-core computer, with several parallel processors, or even a highly parallelized supercomputer, but it was still usually a single computer. The location-centralized matter of computations caused the need to physically move all the data to a single location. Traditional data processing algorithms have been mainly designed for such centralized data processing.

Processed data usually comes from measurements. Since measurements are never absolutely accurate, we must analyze how measurement inaccuracy affects the results of data processing. Traditional algorithm for such analysis – including interval computations algorithms for processing interval uncertainty – have been also mainly designed for centralized data processing.

At present, communications are so fast that with a good connection, it is faster to find the data in someone else's remote operating memory than in one's own disk drive. As a result, it has now become possible to perform computations across the web. It is no longer necessary to move all the data to a centralized location. Instead, we can keep each data set at its place, and use special support software (called cyberinfrastructure) to ease communication between remote computers.

While communications are much faster than in the past, they are still somewhat slower than computations. As a result, when we process distributed data, it is often desirable to modify (and sometimes even redesign) the existing algorithms so as to minimize the amount of communication between remote computers. There has been a lot of progress in developing such cyberinfrastructure-friendly modifications of data processing algorithms. There is a need to extend these modifications to algorithms for processing uncertainty, in particular, to algorithms for processing interval uncertainty.

In this talk, we present several such modifications that we have developed for applications to geosciences and to environmental science. Some of these applications have been described in [1].

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Keywords: cyberinfrastructure, uncertainty, geosciences, environmental science

A Computer-Assisted Band-Gap Proof for 3D Photonic Crystals

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Photonic crystals are optical materials in which light with frequency in certain ranges – the so-called photonic band gaps – cannot propagate, while other frequencies can. Mathematically they are usually modelled by Maxwell's equations (in the frequency domain)

$$\mathrm{curl}E = -i\omega H,\ \mathrm{curl}H = i\omega\varepsilon E,$$

$$\mathrm{div}(\varepsilon E) = 0,\ \mathrm{div}H = 0 \quad (\text{on } \mathbf{R}^3) \tag{1}$$

for the electric field E and the magnetic field H, with $\varepsilon : \mathbf{R}^3 \to \mathbf{R}$ denoting the electric permittivity, a bounded function bounded positively away from zero, which for a photonic crystal is moreover periodic on $\mathbf{R}^3$ with periodicity cell Ω. For simplicity, we assume that $\Omega = (0,1)^3$. ω is the frequency of a monochromatic light wave sent into the crystal, and mathematically it takes the role of a spectral parameter in (1). If ω is in the *spectrum* of (a suitable self-adjoint operator theoretical realization of) problem (1), the light wave can propagate in the crystal; if ω is in the resolvent set, the light wave is absorbed.

By Floquet-Bloch theory, the spectrum σ of (1) is given as a union

$$\sigma = \bigcup_{n=1}^{\infty} I_n \tag{2}$$

of compact real intervals I_n, and in turn each I_n is characterized by

$$I_n = \left\{ \lambda_{k,n} \ :\ k \in [-\pi,\pi]^3 \right\}, \tag{3}$$

where $\lambda_{k,n}$ is the n-th eigenvalue of the semiperiodic eigenvalue problem (to be formulated weakly)

$$\mathrm{curl}\left(\frac{1}{\varepsilon}\mathrm{curl}u\right) = \lambda u \text{ in } \Omega,\ \mathrm{div}u = 0 \text{ in } \Omega,$$

$$u(x+z) = e^{ik\cdot z}u(x)\ (x \in \Omega,\ z \in \mathbf{Z}^3) \tag{4}$$

depending on $k \in [-\pi,\pi]^3$.

Usually, the *spectral bands* I_n in (2) overlap, but it may happen that gaps open between them. These are the band gaps of prohibited frequencies mentioned earlier, and it is of great practical interest to know if they are present or not. Analytically, this question is very difficult to decide.

We will propose a computer-assisted approach for proving the existence of photonic band gaps for specific materials, i.e. for specific permittivity functions ε. We use the characterization (2)-(4) for this purpose, but we have to overcome the problem that *infinitely many* eigenvalue problems (4) have to be treated due to their dependence on $k \in [-\pi,\pi]^3$.

For this purpose, we first choose a finite *grid* G in $[-\pi,\pi]^3$, and compute enclosures for $\lambda_{k,1},\dots\lambda_{k,N}$ (with $N \in \mathbf{N}$ chosen fixed) for all $k \in$ G. This is done by variational eigenvalue

enclosure techniques, more particularly by the Rayleigh-Ritz method (for upper bounds) and the Lehmann-Goerisch method (for lower bounds), supplemented by a homotopy algorithm connecting problem (4) to a simple constant coefficients problem which can be solved in closed form.

Next, we use an explicit *perturbation* argument for self-adjoint operators to bound differences $\left|\lambda_{k,n} - \lambda_{\tilde{k},n}\right|$, for $\tilde{k} \in [-\pi, \pi]^3$, and $k \in \mathrm{G}$ a "nearby" grid point. Altogether, we obtain bounds for $\lambda_{k,1}, \ldots, \lambda_{k,N}$ for *all* $k \in [-\pi, \pi]^3$, and thus, by (3), for the spectral bands $I_1, \ldots, I_N$. If a gap opens between these enclosures, we are done.

The technique described above has been applied successfully to a two-dimensional problem where moreover we restricted ourselves to polarized light waves. Computations for full three-dimensional problems are presently in progress.

Keywords: Photonic crystal, Photonic band-gaps, Computer assisted proof

Application of Order-Preserving Functions to the Modelling of Computational Mechanics Problems with Uncertainty

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In order to efficiently use mathematical models of engineering models it is necessary to know the values of the parameters which describe the models. In this paper the authors will be working on three groups of parameters

1. parameters which can be described by the real numbers (e.g. point loads, displacement of the nodes etc.)

2. parameter which can be described by functions (e.g. distributed loads, density of the materials etc.)

3. parameters which are subsets of R^2 or R^3 (e.g. the shape of the structure).

Unfortunately very often the exact values of these parameters are not known. In such situations it is necessary to use some method for modeling of uncertainty. For parameters which are real numbers it is possible to use intervals [1] (or probability density function). In order to describe the uncertain functional and set parameters it is possible to use interval functions (or stochastic process) and interval sets (or random sets). Functional intervals and interval sets can be defined using partial order relations. According to numerical experiments many solutions for computational mechanics problems are order preserving (i.e. monotone). Hence extreme values of the solutions can be calculated using sensitivity analysis [2]. Unfortunately due to high computational complexity not all general optimization methods can be apply to the solution of complex problems with the interval parameters. If the sign of the difference $f(y) - f(x)$ and $y - x$ is constant (see [3]) then the extreme values of the function can be calculate by using the extreme values of the variable x. Sometimes it is easier to determine the sign of the infinitesimal increments (or differentials) and calculate the extreme values of the solution in the infinitesimal interval. In that case it is possible to extrapolate the results to the case of narrow intervals. Presented approach was applied to the solution of specific problems of structural and fluid mechanics.

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Keywords: interval analysis, uncertainty, reliability, order-preserving functions

On the Theory Behind Interval and Affine Splitting with Extrapolation

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The main drawback of naive interval arithmetic (Natural Interval Extension) is that, it produces conservative bounds. This is because it considers multiple occurrences of same variable in a function as independent of each other. We analyze the cause of this over-estimation in detail. Interval splitting is a method to improve the tightness of the bounds. The method is based on subdivision of intervals and reevaluating the expression. We explore the theoretical basis of extrapolation methods when applied to NIE (Natural Interval Extension) and its effectiveness in predicting the excess width due to over-estimation and hence improving the tightness of bounds. We derive analytical expressions to quantify the effect of extrapolation on excess width due to over-estimation among different classes of polynomial functions. We suggest using higher number of splits for extrapolating excess width due to over-estimation for some classes of functions, so that the width remains small enough, yielding better results with extrapolation. We call this method *Late Start*. We find that the tightness of bounds produced by extrapolation depends to a great extent on the monotonicity of the function, the width of the interval and the method used to perform interval splitting. We prove that monotonic functions perform much better than non-monotonic functions with extrapolation techniques. We identify certain properties of functions that make them good candidates for interval splitting with extrapolation method. We give theoretical proofs to establish the validity of our findings. We prove interval bisection will yield better results with extrapolation than any other methods of interval splitting. Also we explore the effects of extrapolation with higher order terms i.e. coefficients of excess width equation, that depend on the square of the interval width. We analyze the effect of extrapolation technique on affine arithmetic splitting as well. We find affine arithmetic splitting with extrapolation, gives quadratic convergence of prediction coefficients where as interval splitting with extrapolation gives linear convergence. We derive conditions under which affine arithmetic splitting with extrapolation gives better results compared to extrapolation based interval splitting technique. We compare this method with interval splitting and affine arithmetic. We justify the use of extrapolation technique and give theoretical framework for further development of this method.

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Keywords: Interval splitting, Affine splitting, Extrapolation, Late Start, quadratic convergence

Stress Analysis of a Doubly Reinforced Concrete Beam with Uncertain Structural Parameters

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In this paper, the cross-section of a doubly reinforced concrete beam with interval values of structural parameters and subjected to an interval bending moment is taken up for analysis. The uncertainties in loading, areas of reinforcement in tension and compression and the corresponding Young's modulus of steel are defined by fuzzy membership functions. The interval values of the structural parameters at a specified level of uncertainty are extracted from these membership functions using the α-cut approach. The internal moment of resistance of the beam is expressed as a function of interval values of stresses in concrete and steel. The stress distribution model for the cross section of the beam given by IS 456-2000 (Indian Standard Code of Practice for Plain and Reinforced Concrete) is modified for this purpose. The internal moment of resistance is then equated to the external bending moment due to interval loads acting on the beam.

The stresses in concrete and steel are obtained as interval values for various combinations of interval structural parameters. The stress analysis is performed by three principal approaches viz. a search based algorithm, sensitivity analysis and a combinatorial approach. Also, approximate search based solution schemes are applied on the same problem. The reduced optimization performs the search on a subset of the uncertainty space by first identifying the uncertain parameters that have substantial impact on the output of interest. A response surface based method further reduces the computational burden of the global optimization problem. Reference results with guaranteed accuracy are calculated using global optimization.

The methods are compared to the reference results for accuracy as well as numerical efficiency. Combined membership functions are plotted for neutral axis depth and stresses in concrete and steel and are found to be triangular. Interval stresses and strains are also calculated. It is observed that the results obtained are in excellent agreement. These approaches allow the designer to have a detailed knowledge about the effect of uncertainty on the stress distribution of the beam. Thus modelling with intervals provides a link between design and analysis where uncertainty may be represented by bounded sets of parameters.

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Keywords: uncertainty, sensitivity analysis, search-based algorithm, interval stresses and strains

Modeling of Failure Surface of a Reinforced Concrete Slab with Fuzzy Loading – An Interval Approach

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In this paper, a two-way reinforced concrete slab subjected to uncertain loading is analyzed. The uncertainty in loading is defined by a fuzzy membership function. The interval values of load at specified levels of uncertainty are extracted from this membership function using the α-cut approach. Pownuk's sensitivity analysis approach and Muhanna's interval finite element approach are used to determine interval values of generalized displacements of the slab.

Post-processing is performed to obtain the interval stresses in concrete and steel along long span and short span directions of the slab. Fuzzy membership functions of stresses in concrete and steel are obtained by using the procedure suggested by Muhanna and Mullen, Rao and Chen, Moens and Vandepitte.

The interval stresses obtained from the analysis are used to define the interval failure surface. A mathematical model for the interval version of Drucker-Prager yield theory is developed for this purpose. A nested family of interval failure surfaces is utilized to construct a fuzzy membership function for yield surface. Further, the sensitivity of failure surface with reference to corresponding change in loading is evaluated. The present approach allows the designer to have a detailed knowledge about the effect of uncertainty on the stress distribution of the slab and its failure pattern.

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Keywords: uncertainty, sensitivity analysis, α-cut approach, concrete slab, interval stresses, failure surface

Validated Simulation of ODEs and DAEs in ValEncIA-IVP

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ValEncIA-IVP is a validated solver for initial value problems for sets of ordinary differential equations (ODEs) which determines guaranteed enclosures of all reachable states [3]. In this contribution, we present new algorithmic developments extending this solver to a wider class of dynamical system models and improving its performance.

ValEncIA-IVP relies on a simple iteration scheme which can be derived using Banach's fixed-point theorem. Because we describe state enclosures using interval boxes, we, like any other developers of interval software, need techniques to handle typical sources of overestimation: the wrapping effect and multiple dependencies of the iteration formula on common interval variables. To prevent diameters of the interval enclosures from growing for asymptotically stable systems, a new exponential enclosure technique has been derived. This approach allows us to describe solution sets which are contracting over time [4]. A further method to detect and eliminate regions in the state space resulting from overestimation is the consistency test using either backward integration of subintervals or physically motivated dynamical constraints expressing certain conservation properties. Besides, the preconditioning algorithm introduced in [4] has been extended to be applicable to nonlinear problems. This algorithm is based on the transformation of linear systems into real Jordan normal form.

In addition to ODEs, ValEncIA-IVP can be applied to sets of differential-algebraic equations (DAEs). For that purpose, validated solvers for nonlinear algebraic equations have been integrated into its core. For both ODEs and DAEs, routines for validated sensitivity analysis are available. In ValEncIA-IVP, the sensitivities are defined as the partial derivatives of the trajectories of all system states with respect to (uncertain) parameters. The corresponding sensitivity equations are given by sets of ODEs which are derived automatically using algorithmic differentiation provided by FADBAD++ [5].

An important application area of such a validated DAE solver is reachability analysis without symbolic elimination of algebraic constraints. Further, so-called inverse control problems can be handled with its help. In this case, time-dependent algebraic equations in sets of DAEs serve as constraints which specify the desired output signals of a dynamical system [2]. The unknown quantities are the corresponding inputs and the enclosures of the trajectories of the state variables. The prerequisite for both simulation and inverse controller synthesis is that sets of consistent initial values are known.

In contrast to other validated solvers for dynamical systems, ValEncIA-IVP can exploit specific system properties to automatically readjust state enclosures if guaranteed a-priori bounds for them are known (e.g. if state variables are known to be non-negative). Additionally, a validated test for cooperativity is available to tighten the set of solutions [1]. Such properties are typical for a large class of biological and biochemical processes as well as for systems in chemical process engineering.

In conclusion, we derive suitable criteria for the implementation of a scheme for automatic step size control which both reduces the computational effort and allows the user to control the quality of the resulting state enclosures.

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Keywords: Ordinary differential equations, differential-algebraic equations, initial value problems, inverse control problems, VALENCIA-IVP

Detection and Reduction of Overestimation in Guaranteed Simulations of Hamiltonian Systems with Applications in Mechanics

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The dynamics of a large class of mechanical systems, electric circuits, and electro-mechanical components can be described mathematically using sets of canonical equations based on a Hamiltonian formulation of continuous-time state equations [5]. For that purpose, the Hamiltonian $H(q,p)$, which represents the sum of the potential and kinetic energy for mechanical systems, is introduced. The vectors of generalized coordinates q and generalized momenta p can be used to derive the canonical equations

$$\dot{q} = \frac{\partial H(q,p)}{\partial p} = M^{-1}(q) \cdot p$$
$$\dot{p} = -\frac{\partial H(q,p)}{\partial q} + \tau \ ,$$

where $M(q) = M(q)^T$ is the positive definite, symmetric mass matrix and τ the vector of generalized external forces.

In recent years, stability-based techniques for controller design of nonlinear systems significantly gained in importance. The Hamiltonian expresses the total energy of a dynamical system. It can therefore be chosen as a positive definite function and considered as a candidate for a Lyapunov function to prove the stability of a dynamical system. Furthermore, regions of attraction of asymptotically stable equilibria can be derived. In addition, it can be shown that the Hamiltonian system representation provides further information about the dynamics of uncertain systems. This information can be employed efficiently as a constraint in interval-based simulation routines to detect, quantify, and reduce overestimation. For that purpose, a consistency test has been developed to restrict the set of solutions to physically meaningful areas [2].

In this contribution, a computational procedure which derives Hamiltonian constraints automatically is presented. It is applied in efficient validated simulation routines for nonlinear continuous-time systems described by sets of ordinary differential equations. The use of these constraints is demonstrated for applications in mechanical engineering using SmartMOBILE [1] as a validated modeling and simulation software for multibody systems with ValEncIA-IVP [4] as the underlying integration algorithm. In this example, the Hamiltonian of a closed mechanical system without any gain or loss of energy is considered.

However, the above-mentioned Hamiltonian constraints might fail to detect a portion of overestimation, if they do not depend on the state variables introducing it. To solve this problem, further constraints based on specific physical system properties such as the energy conservation law or mass balance equations have to be derived. This extension allows us to generalize the consistency test for use in various applications in engineering, medicine, and biology.

In general, constraints for dynamical systems can be classified into holonomic and non-holonomic [3]. Holonomic ones can be expressed as algebraic functions $g(q,t) = 0$ depending upon the time variable t and the generalized coordinates q. All other constraints which cannot be represented in this form, e.g. inequalities or constraints depending on the velocity $\dot{q}$, are non-holonomic. We use representative system models to demonstrate the necessity to use both types to restrict the set of possible solutions. Simulation results show how suitable constraints can be chosen to obtain state enclosures which are as tight as possible.

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Keywords: Hamiltonian systems, constraints, consistency tests, ValEncIA-IVP, SmartMOBILE

Robust and Optimal Control of Uncertain Dynamical Systems with State-Dependent Switchings Using Interval Arithmetic

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In this contribution, interval arithmetic techniques for controller design of nonlinear dynamical systems with uncertainties are summarized. The main reason for the application of interval techniques in this context is the quantification of the influence of uncertainties and modeling errors. They result from neglecting nonlinear phenomena in the mathematical description of real-world systems. Furthermore, measured data usually do not provide exact information about the systems' parameters. Often simplifications of nonlinear models or controller structures are necessary to enable their implementation.

In the first part, techniques for verification of controllability, reachability, and observability of states in the presence of uncertainties as well as stabilizability of instable systems are demonstrated. These techniques are based on the validated evaluation of the corresponding system theoretic criteria [1]. Therefore, computational approaches are applied which yield guaranteed enclosures of all reachable states of dynamical systems. Especially for safety-critical applications, the systems' asymptotic stability and compliance with given restrictions for the state variables have to be assured for all possible operating conditions using analytical or numerical techniques. For both open-loop and closed-loop control systems, possibilities for combination of validated techniques with classical approaches for robust and stability-based controller design in the time-domain and frequency-domain are highlighted.

In the second part, procedures for structure and parameter optimization of continuous-time dynamical systems with bounded uncertainties are derived which rely on the above-mentioned basic concepts [5]. After an overview of both validated and non-validated numerical routines which are applicable for that purpose [2,3], an interval-based algorithm is presented, which computes approximations of globally optimal open-loop and closed-loop control laws for both discrete-time and continuous-time systems. Focusing on continuous-time applications, we present new strategies which allow to combine piecewise constant approximations of optimal control laws with continuous approximations.

The focus of the third part is the application of the previously introduced methods and procedures to the design of robust and optimal control strategies for dynamical systems with state-dependent switching characteristics [5]. In practically relevant application, the fact that control variables are usually bounded has to be taken into account directly during the design stage. This aims at building a new unified, general-purpose framework for the validated synthesis of dynamical systems integrating trajectory planning, function-oriented and safety-related controller design, as well as robustness and optimality assessment and verification. Computational routines for the

previously mentioned tasks already exist. However, they are usually not integrated into a common tool verifying the design using interval arithmetic.

Finally, using interval methods, the potential of approximation techniques which gain more and more importance in modern approaches for controller design can be analyzed. Approximation techniques often provide necessary information on how to choose appropriate structures of parameterizable control laws for nonlinear processes [4,6]. However, in most cases, the analysis of the resulting control laws with respect to parameter variations and approximation errors is inevitable since these uncertainties might heavily influence the stability of the closed-loop system.

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Keywords: Interval arithmetic, controller design, optimization, approximation techniques, safety-critical applications

Transaction Modeling for Distributed High Performance Computing

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Distributed transaction design and optimization for clustered high-performance computing ("CHPC") environments are impacted by node transaction processing times and network bandwidth and latency. To better understand the impact of competing designs, transaction processing times must be accurately represented. While representations based on a given probability density distribution, such as the exponential density, may offer acceptable approximations for processing times of short-lived, low volume node transactions, a more realistic type of representation is needed for long-lived, high-volume CHPC transactions mainly due to the large-scale volume effect of multimodality of actual processing time density distributions. In this paper we present modeling analysis for transaction processing times and we propose use of mixture distributions as a generalized representation for simulation of CHPC distributed transactions [1,4,5]. Modeling and simulation perspectives are presented from the point of view of transaction design, as opposed to the point of view of network design which models transactions as aggregate network traffic [2,3]. Transaction design and optimization in CHPC environments are critical because typical applications saturate the system interconnect network [6]. A naive transaction design, one which does not consider the performance impact of a network that operates in saturation during the steady-state phase of the processing, is appropriate for initial application development, but it must be replaced by a performance-tuned design for production. Our analysis is based on a three-node multithreaded model which is naturally generalized into a high-performance distributed design.

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Global Optimization and Ill-Posed Nonlinear Programs: New Techniques

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We consider the general nonlinear program

$$\boxed{\begin{array}{l}\text{minimize } \phi(x)\\ \text{subject to } c_i(x) = 0,\ i = 1, \ldots, m_1,\\ \qquad\qquad g_i(x) \le 0,\ i = 1, \ldots, m_2,\\ \text{where } \phi : \boldsymbol{x} \to \mathbb{R} \text{ and } c_i, g_i : \boldsymbol{x} \to \mathbb{R}, \text{ and where}\\ \boldsymbol{x} \subset \mathbb{R}^n \text{ is the hyperrectangle (box) defined by}\\ \qquad\qquad \underline{x}_i \le x_i \le \overline{x}_i,\ 1 \le i \le n,\\ \text{where the } \underline{x}_i \text{ and } \overline{x}_i \text{ delineate the search region.}\end{array}} \tag{1}$$

Both linear and nonlinear programs are often approximately ill-posed, with an entire continuum of approximate optimizing points. As an example, take the linear program

Minimize $10A + 3.5B + 4C + 3.2D$

Subject to:

$$\begin{array}{rcrcl} 100A + 50B + & & 80C + 40D & \le & 200,000,\\ 12A + & & 4B + 4.8C + & 4D \ge & 18,000,\\ 0 & \le & 100A & \le & 100000,\\ 0 & \le & 50B & \le & 100000,\\ 0 & \le & 80C & \le & 100000,\\ 0 & \le & 40D & \le & 100000, \end{array}$$

which we derived in [1] from a simple investment scenario. Any point along the portion of the line $B = 0$, $D = 2500$, A and C given parametrically by

$$\begin{pmatrix} A \\ C \end{pmatrix} \approx \begin{pmatrix} 666.\overline{6} \\ 0 \end{pmatrix} + t \begin{pmatrix} -0.3714 \\ 0.9285 \end{pmatrix},$$

with $0 \le C \le 1250$, is a solution to this problem. If we perturb the coefficients of this problem slightly, we might obtain

Minimize $10.1A + 3.5B + 4.08C + 3.2D$

Subject to:

$$\begin{array}{rcrcl} 100A + 50B + & & 80C + 40D & \le & 200,000,\\ 12.4A + & & 4B + 4.88C + & 4D \ge & 18,000,\\ 0 & \le & 100A & \le & 100000,\\ 0 & \le & 50B & \le & 100000,\\ 0 & \le & 80C & \le & 100000,\\ 0 & \le & 40D & \le & 100000. \end{array}$$

This new problem has a unique solution at $A \approx 645.161$, $B = C = 0$, $D = 2500$. However, the perturbed problem inherits a set of *approximate* solutions along a portion of the line given parametrically by

$$\begin{pmatrix} A \\ C \end{pmatrix} \approx \begin{pmatrix} 645.161 \\ 0 \end{pmatrix} + t \begin{pmatrix} -0.3669 \\ 0.9302 \end{pmatrix}.$$

In both the exactly singular case and the approximately singular case, we obtain the parametric representation of the solution set (or the approximate solution set) from a singular value decomposition of the matrix of gradients of the objective and active constraints, although, in the approximately singular case, more constraints are active, and we need to explore by selectively removing some constraints to find directions in which feasibility is maintained.

Although it can be practical to know, commercial software doesn't always detect such manifolds of solutions, as we have illustrated in [1]. In [1], we considered a skewed coordinate system, with orthogonal coordinates aligned with the null space of the objective and constraint gradients, and an epsilon-inflation process for eliminating large volumes around such a degenerate solution set of the optimization problem. However, our examples there were exclusively linear. Furthermore, there are various issues on how to incorporate the epsilon-inflation process into rigorous exhaustive search algorithms, such as how to use the tessellation in the skewed coordinate system within a branch and bound process carried out in the original coordinate system. We will report progress in these areas, as appropriate.

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Constraint Programming and Safe Global Optimization

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Interval methods have shown their ability to locate and prove the existence of a global optima in a safe and rigorous way but these methods are rather slow. We investigate the capabilities of constraints techniques to boost these methods, and thus, to reduce the gap between efficient but unsafe systems like Baron, and slow but safe global optimization approaches.

First, we study the capabilities of consistency techniques to speed up the initial convergence of the interval narrowing algorithms. We show how linear relaxations can be used in such a CP framework to rigorously bound the global optima as well as its location. Second, we show how constraint programming filtering techniques can be used to implement optimality-based reduction in a safe and efficient way, and thus to take advantage of the known bounds of the objective function to reduce the domain of the variables, and to speed up the search of a global optimum.

Finally, we introduce a new strategy to compute very accurate approximations of feasible points. This strategy takes advantage of the Newton method for under-constrained systems of equations and inequalities to compute efficiently a promising upper bound. Experiments on the Coconuts benchmarks demonstrate that these different techniques drastically improve the performances.

A Multiresolution Scheme for the Bidomain Model in Electrocardiology

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Since direct measurements represent an obvious difficulty in electro-cardiology, there exists a wide interest in the numerical simulations of cardiac models. Here we present a finite volume method enriched with a fully adaptive multiresolution scheme, a Runge-Kutta-Fehlberg adaptive scheme, and a locally varying time stepping, for solving the widely known monodomain and bidomain equations modeling the electrical activity of the myocardial tissue. The bidomain model, is a degenerate parabolic PDE for the so-called transmembrane potential, which is coupled with an elliptic PDE for the extracellular potential, and involves a time-dependent ODE for the so-called gating variable; in the simpler sub-case of the monodomain model, the elliptic PDE reduces to an algebraic equation. Two simple models for the membrane and ionic currents are considered, one proposed by Mitchell and Schaeffer [1] and the simple FitzHugh-Nagumo model [2]. The bidomain model represents a computational challenge since the width of an excitation front is about two orders of magnitude smaller than the long axis of a human-size right ventricle. This local feature, along with strongly varying time scales in the reaction terms, causes solutions to produce sharp propagating wave fronts in the potential field, which almost precludes simulations with uniform grids. Clearly, cardiac simulations should be based on space- (and also time-) adaptive methods.

We firstly prove, following [3], well-posedness for a class of these problems consisting in a strongly coupled and degenerate parabolic-elliptic system. We also prove existence, uniqueness of approximate solution and convergence of the numerical scheme to the corresponding weak solution, obtaining in this way, an alternative proof for the well-posedness result. As in [4], After introducing the multiresolution technique, an optimal threshold for discarding non-significant information is derived and the efficiency and accuracy of the numerical method is viewed in terms of CPU time speed-up, memory compression and errors in different norms.

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Keywords: Bidomain model, degenerate reaction-diffusion system, fully adaptive multiresolution schemes, Runge-Kutta-Fehlberg, local time stepping

Error-Free Transformations and Applications

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Recently there is quite some interest in so-called error-free transformations. For two given floating-point numbers a, b those transform it into a new pair x, y of floating-point numbers such that the first one x is the result of a floating-point operation and the second y is the exact error. For example, $a * b = x + y$ with $x = fl(a * b)$. Using error-free transformations we developed the currently fastest summation and dot product algorithms (joint work with Ogita and Oishi). In this talk we present some new applications, among them the computation of predecessor and successor of a floating-point number. This can be used to simulate interval operations in rounding to nearest.

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From Linear to Branching Time in Software Property Specifications

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Software verification is a fundamental part of the software development process. Formal verification techniques, such as runtime-monitoring [4] and model checking [1], are based on formal specifications of software behavior.

Temporal logic is one of the most widely used form of specifying system properties. It is the branch of logic that enables practitioners to establish causal and temporal relations between propositions. Formulas in temporal logic depend on time, i.e., the truth value of a particular temporal logic formula depends upon the order of states. Linear Temporal Logic (LTL) and Computational Tree Logic (CTL) are the two most commonly used types of temporal logic in property specifications because of their high expressibility. Both logics are subsets of the temporal logic CTL*.

Both LTL and CTL use the traditional Boolean operators for conjunction, disjunction, negation, and implication. In addition, they use a series of operators to temporally relate propositions within their respective statements. States in LTL are represented using a linear sequence. On the other hand, states in a CTL specification represent a tree. As mentioned above, both logics use the same set of logical operators. However, CTL adds the quantifiers $\forall$ and $\exists$ to specify all paths or a single path respectively.

While it is the case that each of LTL and CTL can express properties that the other logic cannot, it is believed that most software properties lie in the intersection of the two logics. It is generally accepted that LTL is more intuitive and easier to use, while CTL is believed to be easier to formally verify [7].

Creating and validating formal specifications in either logic is a significant impediment to the adoption of formal verification techniques [3]. There have been successful research efforts to minimize the challenges of creating formal specifications including the Specification Pattern System (SPS) [2] and Composite Propositions (CPs) [5]. These approaches assist a user in the creation of specifications based on the notions of patterns and scopes. Patterns represent templates of commonly used software properties. Scopes define the limits of program execution over which a pattern is to be evaluated. Each pattern or scope has a set of parameters (defined by propositions) that define the beginning and end moments of time (i.e. program states) over which the pattern or scope is valid. CPs allow the user to define a pattern or scope parameter using multiple propositions.

Defining LTL or CTL formulas for all patterns (five patterns), scopes (five scopes), and CPs (eight CP classes) requires the generation of a large amount of complex specifications. In recent research efforts we were able to develop a set of LTL specification templates that support SPS patterns and scopes and CPs [6]. This work reports on the effort to use these LTL templates as a base to generate similar CTL templates. In other words, we attempt to answer the following questions; Do the specifications defined by the templates in [6] belong to the intersection of LTL

and CTL? and if so, is there a simple way of translating these templates into the equivalent CTL ones?

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Keywords: Formal Specifications, LTL, CTL, Patterns, Scopes, Composite Propositions.

On the Shape of the Solution Set Concerning a Linear Complementarity Problem with Interval Data

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Given a vector $q \in \mathrm{R}^n$ and a matrix $M \in \mathrm{R}^{n\times n}$ the linear complementarity problem (LCP) is to find a vector z such that

$$q + Mz \geq o, \quad z \geq o, \quad (q + Mz)^{\mathrm{T}} z = 0, \tag{1}$$

or to show that no such vector exists; here, the $\geq$-sign is meant componentwise. The LCP has many applications; see [3] and [4]. In [5] we considered an LCP where the input data q and M are not exactly known but can be enclosed in intervals. This generalization arises from discretizing a free boundary problem and taking into account the discretization error.

This means, we have an interval vector $[q] \in \mathbf{IR}^n$ and an interval matrix $[M] \in \mathbf{IR}^{n\times n}$, and we are interested in an enclosure method for the solution set

$$\Sigma([q],[M]) := \{z \in \mathbf{IR^n} : \exists \mathbf{q} \in [\mathbf{q}],\, \mathbf{M} \in [\mathbf{M}] \text{ with } (\mathbf{1})\};$$

see [1]. If every $M \in [M]$ is a M(inkowski)-matrix, which means that every $M = (m_{ij}) \in [M]$ is regular satisfying $m_{ij} \leq 0$ for $i \neq j$ and $M^{-1} \geq O$, then we have shown in [1] that

$$\inf \Sigma([q],[M]) \in \Sigma([q],[M]) \quad \text{and} \quad \sup \Sigma([q],[M]) \in \Sigma([q],[M])$$

hold. The assumption, that every $M \in [M]$ is an M-matrix, is satisfied in the application from [5].

A question naturally arises: What does the solution set $\Sigma([q],[M])$ actually look like? We give an answer to this question and we present some new insight concerning enclosure methods for $\Sigma([q],[M])$.

We present two sequences of vectors $\{x^{(k)}\}$ and $\{y^{(k)}\}$ such that

$$x^{(0)} \leq x^{(1)} \leq ... \leq x^{(k)} \leq y^{(k)} \leq ... \leq y^{(1)} \leq y^{(0)}$$

and

$$\lim_{k\to\infty} x^{(k)} = \inf \Sigma([q],[M]) \quad \text{and} \quad \lim_{k\to\infty} y^{(k)} = \sup \Sigma([q],[M])$$

hold for the case that every $M \in [M]$ is an M-matrix.

Finally, we will emphasize a difference between $\Sigma([q],[M])$ and the solution set

$$S([b],[A]) := \{x = A^{-1}b : b \in [b],\, A \in [A]\}$$

arising from interval linear systems of equations considered in [2].

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Probabilistic and Interval Uncertainty of the Results of Data Fusion, With Application to Geosciences

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In many real-life situations, we have several measurements and/or expert estimates $u_1, \ldots, u_n$ of the same quantity u. In such situations, it is desirable to fuse the resulting estimates into a single more accurate estimate. When each u_i is known with interval uncertainty, i.e., when we know the interval $\mathbf{u}_i = [u_i - \Delta_i, u_i + \Delta_i]$ containing the actual (unknown) value of u, then u belongs to the intersection $\mathbf{u} \stackrel{\text{def}}{=} \bigcap_{i=1}^{n} \mathbf{u}_i$ of these intervals. When each u_i is known with probabilistic uncertainty, e.g., when the measurement error $\Delta u_i \stackrel{\text{def}}{=} u_i - u$ is normally distributed with 0 mean and known standard deviation σ_i, then we can use the Least Squares Method (LSM) to combine u_i into a more accurate estimate $\widetilde{u}$ for u; see, e.g., [1].

In many practical situations, however, different measurements have not only different accuracy, but also different resolution. For example, in the geosciences, seismic data leads to higher-resolution estimates of the density at different locations and depths, while gravity data leads to lower-estimates of the same densities. In precise terms, we have high-resolution estimates $\widetilde{u}_1, \ldots, \widetilde{u}_n$ of the density values $u_1, \ldots, u_n$ within several small spatial cells, and we also have a low-resolution estimate $\widetilde{u}$ for the weighted average $u = \sum_{i=1}^{n} w_i \cdot u_i$.

We are interested in the densities themselves and in auxiliary quantities q (such as expected amount of oil in an oil field) that can be estimated based of these densities. So, based on the estimates $\widetilde{u}_i$ and $\widetilde{u}$, we must provide more accurate estimates for the quantities u_i themselves and for the auxiliary quantities $q = f(u_1, \ldots, u_n)$ depending on u_i.

In this talk, we describe how to compute such fused estimates. In the probabilistic case, we use LSM to derive explicit formulas for combining the estimates $\widetilde{u}_i$ and $\widetilde{u}$. In the interval case, we provide an efficient algorithm for estimating the ranges of u_i and q.

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Parameter Characterization of Linear Time-Varying Models: An Optimal Solution

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A method is proposed for optimal parameter characterization of a linear model derived from the transfer function of a complex dynamic system (CDS). Describing complex industrial processes generally leads to mathematical models of very high order. Examples of these processes are mobile arc welding robot or wood cutting system [8]. These models are very time-consuming from processing point of view. Therefore, from an engineering point of view, one is more interested in manipulating a simpler and consequently less accurate mathematical model rather than a complex and more accurate one. In this objective, simplification is performed using model reduction methods [7]. Having been simplified, the model describes system's response less accurately and hence, there is generally a difference between observed and estimated values which is called *modeling error*.

Handling modeling error is among the most challenging problems in almost all identification procedures in control engineering. Classical method is the probabilistic approach in which model's parameter vector φ is optimized with respect to a given criterion and modeling error is characterized by means of a certain Probability Density Function (PDF) [2]. Another alternative is the set-membership approach in which parameter vector φ is supposed not to be precisely known but restricted to a given set. Possible Parameter Set (PPS) is then characterized by interval vector $[\varphi]$ and as a result, the model produces a tube called *wrapping envelope* for system's response [3,5]. It is then guaranteed that the wrapping envelope includes all possible values of system's responses while considering variation of system's behaviour in time, simplified model structure and perturbations. This fundamental property is the main motivation to explore the set membership approach to describe dynamic systems in critical industrial applications in which one needs guaranteed results. To improve the precision of wrapping envelope, i.e. to obtain a thinner envelope, other convex geometrical shapes such as zonotope [1], polytope [6], and ellipsoid [4] have been exploited to characterize PPS; the shape is pre-defined whereas its size is subject to further tuning to optimize the given criterion.

Contrary to previous methodologies in which the shape of PPS is predefined and system's observations are utilized to tune its size, this work proposes a piecewise parameter identification method which consists of two main steps. In the first step, numerical value of parameter vector φ_k is calculated at any instant such that the model describes the system's response precisely. Set $PPS = \{\forall k | \varphi_k\}$ determines a volume in parameter space which in the second step, is characterized by its convex hull H_S. The latter is the subset of any other convex geometrical shapes (zonotoe, polytope, elipsoid) characterizing PPS. Considering inclusion property, the image of H_S is a subset of the images of the other shapes with respect to linear transformation of the model, i.e. the wrapping envelope produced by using convex hull H_S is included in the envelopes produced by using the alternative shapes. H_S is optimal with respect to the width of wrapping envelope as optimization criterion.

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Keywords: Time-Varying Systems, Parameter Characterization, Set-Membership Approach, Interval Analysis

Tolerable Solution Sets of Interval Linear Systems with Dependent Data

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We consider interval linear systems of the form $\boldsymbol{A}x = \boldsymbol{b}$ with interval matrices $\boldsymbol{A} \in \mathbb{IR}^{m\times n}$ and interval right-hand side vectors $\boldsymbol{b} \in \mathbb{IR}^m$, the interval system being understood as a family of point linear systems $Ax = b$ with $A \in \boldsymbol{A}$ and $b \in \boldsymbol{b}$. The coefficients of the system $\boldsymbol{A}x = \boldsymbol{b}$ are said to be *dependent* (or *tied*) provided that the set $\mathcal{A} \subseteq \mathbb{R}^{m\times n}$ from which the point matrices A can take values does not coincide with $\boldsymbol{A}$ (i.e., it is less than $\boldsymbol{A}$).

We define *dependence* (*tie*) between the coefficients as a description (in any form) that enables one to specify the actual set of point matrices $\mathcal{A}$, allowed by the problem statement, from the set of all possible point matrices $\boldsymbol{A}$. Below, it is assumed that a subset $S \subseteq \mathbb{R}^{m\times n}$ is given that expresses a global requirement on the coefficients of the system (elements of the matrix A), while $\mathcal{A} = \boldsymbol{A} \cap \mathcal{S}$. In particular, if no dependence is imposed on the coefficients then we set $S = \mathbb{R}^{m\times n}$.

Definition. Tolerable solution set of the interval linear system $\boldsymbol{A}x = \boldsymbol{b}$ with the dependence (tie) S on the coefficients *is the set of all such vectors* $x \in \mathbb{R}^n$ *that the value* Ax *belongs to the interval* $\boldsymbol{b}$ *for every point matrix* A *from* $\boldsymbol{A} \cap S$*, i.e.*

$$\Xi_{tol}(\boldsymbol{A}, S, \boldsymbol{b}) := \left\{ x \in \mathbb{R}^n \;\middle|\; \bigcup_{A\in(\boldsymbol{A}\cap S)} Ax \subseteq \boldsymbol{b} \right\}.$$

The tolerable solution set of the system $\boldsymbol{A}x = \boldsymbol{b}$ without ties is known to coincide with the solution set of the inclusion $\boldsymbol{A}x \subseteq \boldsymbol{b}$. It is proven in [1] that such solution set may be described by the system of two-sided point inequalities $\underline{\boldsymbol{b}}_i \le ax \le \overline{\boldsymbol{b}}_i$, where the real vector-row a passes through the set of vertices of the interval row $\boldsymbol{A}_{i:}$ and the index i takes values from 1 to m, i.e.

$$\Xi_{tol}(\boldsymbol{A}, \boldsymbol{b}) = \left\{ x \in \mathbb{R}^n \;\middle|\; \bigcup_{A\in\boldsymbol{A}} Ax \subseteq \boldsymbol{b} \right\} = \left\{ x \in \mathbb{R}^n \;\middle|\; \boldsymbol{A}x \subseteq \boldsymbol{b} \right\}$$

$$= \bigcap_{i=1,\dots,m} \bigcap_{a\in \operatorname{vert} \boldsymbol{A}_{i:}} \left\{ x \in \mathbb{R}^n \mid \underline{\boldsymbol{b}}_i \le ax \le \overline{\boldsymbol{b}}_i \right\},$$

$$\operatorname{vert} \boldsymbol{A}_{i:} = \left\{ a \in \mathbb{R}^n \mid a_j \in \{\underline{A}_{ij}, \overline{A}_{ij}\},\ j = 1, \dots, n \right\}.$$

In present work, we propose a method for finding the tolerable solution set of the system $\boldsymbol{A}x = \boldsymbol{b}$ with affine ties between coefficients. The essence of the method is a conversion of the original problem to a system of two-sided point inequalities.

Simplified versions of the method are given for special cases of the affine ties:

1. Let S be a set of point matrices with groups of proportional elements, each group containing no more than one element from every row of the matrix (in particular, S may be one of the

following sets of matrices: symmetric, skew-symmetric, Toeplitz, Hankel, Hurwitz, circulant). Then

$$\Xi_{tol}(\boldsymbol{A}, S, \boldsymbol{b}) = \Big\{ x \in \mathbb{R}^n \;\Big|\; \widetilde{\boldsymbol{A}} x \subseteq \boldsymbol{b} \Big\},$$

where $\widetilde{\boldsymbol{A}}$ is a maximal (with respect to inclusion) interval matrix, such that

- it is a subset of $\boldsymbol{A}$,
- its elements are in the relation assigned for point matrices by the global tie S.

(For example, if S is the set of symmetric matrices, then $\widetilde{\boldsymbol{A}}$ is maximal symmetric interval matrix within the set $\boldsymbol{A}$.)

2. The tolerable solution set of the interval linear matrix equation $\boldsymbol{A}X + X\boldsymbol{B} = \boldsymbol{C}$ may be found from the interval inclusion $\boldsymbol{A}X + X\boldsymbol{B} \subseteq \boldsymbol{C}$.

In both examples, the original problem with dependent coefficients is converted into a similar problem without ties on coefficients. In its turn, the problems with independent input data can be successfully solved by the elaborated techniques from [1,2,3].

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Keywords: interval linear equations, tolerable solution set, dependent (tied) parameters

Nonnegative Interval Linear Equations and Their Solution

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The subject of our presentation is interval linear systems of equations of the form

$$\boldsymbol{A}x = \boldsymbol{b}, \qquad (*)$$

with an interval $m \times n$-matrix $\boldsymbol{A} = (\boldsymbol{a}_{ij})$ and interval right-hand side m-vector $\boldsymbol{b} = (\boldsymbol{b}_i)$. We consider them as collections of usual (point) systems of equations of the form $Ax = b$ of the same structure as $(*)$, whose matrix elements a_{ij} and right-hand side components b_i may independently vary within the intervals $\boldsymbol{a}_{ij}$ and $\boldsymbol{b}_i$ respectively.

For interval linear systems $(*)$, various definitions of solutions and solution sets exist, which lead to various problem statement (see, e.g., [3]). Since the structure of the solution sets is usually quite complex and their direct description may grow exponentially with the dimension of the system, users traditionally confine themselves to computing estimates, in this or that sense, for the solution sets. For instance, inner estimation (by subsets) of the solution sets to interval equations systems is popular in identification under interval uncertainty, while outer interval estimates (by enclosures) are necessary in sensitivity-like analysis.

In the present work, we consider interval linear systems with nonnegative matrices and show that the corresponding solution sets possess *shape monotonicity*, which radically simplifies their study and estimation. In particular, this enables one to construct inclusion-maximal boxes within the solution sets [2].

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Keywords: interval linear equations, nonnegative matrices, solution sets, shape monotonicity

The Non-Numerical Ranking Preferences Method: A Method for the Post-Pareto Analysis of Multiple Objective Problems

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The solution of a multiple objective optimization problem involves three stages: (1) formulation, (2) search, and (3) decision-making. Knowing the solutions contained in the Pareto-optimal set does not completely solve the multiple objective optimization problem, since the decision-maker still has to choose a single solution from this set to be implemented. The method presented is focused on the decision-making stage. This third stage is key in the solution of a multiple objective optimization problem, since having the Pareto-optimal set can sometimes be overwhelming for the decision-maker. Many practitioners (not skilled in utility theory) do not really know how to approach this set, particularly when it is often very large. Therefore, there is a need to provide the decision maker helpful methods that simplify the analysis during the post-Pareto analysis phase.

Although, several methods for solving multi-objective optimization problems have been developed and studied, little prior work has been done on the evaluation of results obtained in multiple objective optimization. The post-Pareto analysis and the selection of one solution over the others may be quite a challenging problem since in the absence of subjective or judgmental information, none of the corresponding trade-offs can be said to be better than the others.

In the present research, the non-numerical ranking preferences method is introduced to narrow the size of the Pareto-optimal set and thus, provide the decision-maker a workable size set of solutions, called the pruned Pareto set. In this method, the objective functions are scaled and then ranked non-numerically by the decision maker. Based on the rankings, an n-dimensional uncertain weight function is developed (similar to a joint distribution function), indicating the likelihood of different weight combinations.

This method is appropriate for decision-makers that understand the objective function preferences to use but cannot select specific w_i values. For the analysis of the solutions of a multiple objective problem, it is very realistic to think that decision-makers can prioritize the objectives, but cannot mathematically combine them, and the formulation presented may be one of the most relevant to solve those classes of problems.

In summary, the strength of this method is precisely that the decision-maker only ranks non-numerically (in order of relative importance) the objective functions but does not have to select specific weight values. This uncertain weight function is generated based on the decision-maker objective function preferences. Possible weight combinations reflecting the decision-makers preferences are generated numerous times from the uncertain weight function. This method has been observed to achieve a 90% reduction of the entire Pareto-optimal set

Solving Decidability Problems with Interval Arithmetic

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An affine iterated function system (IFS, [1]) over the reals is given by a set of contractive affine transformations on a complete metric space $\mathbb{R}^k$ for some positive natural number k. Thus an interesting problem is to decide, whether a given matrix A describes a contraction mapping, i.e. whether there exists some $s < 1$ such that $|Az| \leq s|z|$ for each $z \in \mathbb{R}^k$, where $|\cdot|$ denotes the Euclidean norm. Using the characteristic polynomial and interval methods we can prove the decidability of the contraction mapping property for square matrices over the rational numbers. Let

$$p(x) = \sum_{i=0}^{n} c_i x^i$$

denote a polynomial of degree n. Assume that p has only single roots and that we have computed a set of n real intervals $I_1, \ldots, I_n$ and have proved for each interval that it contains a root of p using the intermediate value theorem. It is easy to see that this is possible using bisection. Then we know that the real interval coefficient polynomial given by

$$P(X) = \prod_{j=1}^{n} (x - I_n) = \sum_{j=0}^{n} C_n x^j$$

satisfies the constraints

1. $p(x) \in P(X)$ for each real interval X and $x \in X$ and
2. $c_j \in C_j$ for each $j = 0, \ldots, n$.

If p has multiple roots, then the situation is only slightly more complicated. We can use interval bisection to compute a set of intervals $I_1, \ldots, I_m$ such that $0 \in p(I_j)$ and the diameter of each interval I_j is at most 2^{-k} for each $k \in \mathbb{N}$. Now each such interval I_j possibly contains a root. There is however at least one choice $t = (i_1, i_2, \ldots, i_m) \in \mathbb{N}^m$ such that

1. $\sum_{j=1}^{m} i_j = n$ and
2. $\prod_{j=1}^{n} (x - I_j)^{i_j} = \sum_{j=0}^{n} C_j x^j$ such that $c_j \in C_j$ for $j = 0, \ldots, n$.

If an m-tuple t satisfies these constraints for the intervals $I_1, \ldots, I_m$, then we say that $(t, I_1, \ldots, I_m)$ generates p. If there exists some m-tuple t for the intervals $I_1, \ldots, I_m$ such that $(t, I_1, \ldots, I_m)$ generates p, then we say that the set $\{I_1, \ldots, I_m\}$ is able to generate p.

Assume that we are given a polynomial p such that p has only rational coefficients and all roots of p are real numbers. We want to decide, whether all roots of p are smaller than a given rational

number d. We can decide, whether d is a root of p by evaluating p for d. Assume the non-trivial case where d is not a root of p. We can compute a root bound interval $[-b, b]$ for some rational number b such that all roots of p are contained in $[-b, b]$. In the following, we will use two sequences of interval sets L_i and R_i, where $L_0 = \{[-b, d]\}$ and $R_0 = \{[b, d]\}$. The sets L_{i+1} and R_{i+1} are obtained from L_i and R_i, respectively, by bisecting the contained intervals and keeping only these, which have an interval evaluation of p containing zero. If we find an i, for which $R_i = \emptyset$, then clearly all roots of p are smaller than d. If, on the other hand, there is some i, such that L_i can no longer generate p, then there exists some root of p which is greater than d. In the paper we show that one of the two cases always occurs. As an optimization, the bisection can be enriched by an application of the interval Newton method.

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Keywords: decidability, interval Newton, interval bisection

Comparison of Pruning Tests for Interval B&B Global Optimization Methods

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Several pruning tests have been proposed for Interval Branch and Bound methods for global optimization. The main idea of these pruning tests is to build a linear lower bounding function for the objective function using gradient information [3,5], although the use of slopes or Lipschitz constants has also been proposed (see [1,2,4]). The regions where the linear lower bounding function is greater than the best upper bound of the global minimum cannot contain any global minimizer point, thus they can be eliminated. The methods differ in the way they construct the linear lower bounding function, which determines the regions that can be pruned out. None of these techniques is clearly superior to other: the average speedup that can be obtained with them is sometimes quite similar, and depending on the problem a given technique may work better than the others.

In this work we compare the two pruning techniques described in, correspondingly, [3] and [5], and aim to design a new pruning method that combines the advantages of both techniques.

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Keywords: global optimization, interval Branch and Bound, pruning tests

A Box-Consistency Contraction Operator Based on Extremal Functions

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Interval-based solving techniques use different operators to compute, in a reliable way, the real solutions of a system of equations. Some *contraction* operators come from the constraint programming community. Starting from an initial search interval for every unknown, contraction operators reduce these intervals and finally converge onto a *box* that contains all the solutions of the system. The state-of-the-art operators `HC4` [1] and `Box-consistency` [1] consider a single equation of the system at each step, and propagate the obtained reductions in the rest of the system until no interval can be reduced.

We consider a particular equation $f(a,x)=0$ of a given system. The $n-1$ first variables of $f : I\!R^{n-1} \times I\!R \rightarrow I\!R$ have been agregated into a vectorial variable $a \in I\!R^{n-1}$. `BoxRevise` (also known as BoxNarrow) is the atomic procedure used by `Box-consistency`. Starting from an initial interval $[x]$ for x, `BoxRevise` computes a reduced interval $[l,r]$ for x with no loss of solution (i.e., $\forall x_s \in [x]\ s.t.\ x_s \notin [l,r], \forall a_s \in [a] : f(a_s,x_s) \neq 0$, $[a]$ being the initial box of a). In practice, `BoxRevise` works with $f([a],x)$, the multivalued function defined on a single variable x obtained by replacing a by the box/interval $[a]$. It computes l (respectively r) as the leftmost (respectively the rightmost) root of $f([a],x)=0$.

Following the latest version `BC4` [1] of `Box-consistency`, if the analytic expression $f(a,x)$ contains only one occurrence of x, the well-known `HC4Revise` narrowing operator [1] computes $[l,r]$ very quickly. Otherwise, `BoxRevise` calls iteratively bisection steps on $[x]$ and univariate interval Newton to compute l (respectively r). This process may converge slowly because $f([a],x)$ is a *multivalued* ("thick") function.

The `PolyBox` (*polynomial Box-consistency*) operator proposed in this paper implements a more efficient `BoxRevise` procedure when $f([a],x)$ satisfies some conditions. These conditions apply for example when $f([a],x)$ is a polynomial. We focus on the polynomial case in this abstract. `PolyBox` first performs symbolic manipulations to rewrite $f([a],x)$ as $g_{[a]}(x) = \sum_{i=0}^{i=d} f_i([a]).x^i$. This step is crucial since the "thickness" of $f([a],x)$ depends on its symbolic form.

We define the *extremal functions* as $\underline{g_{[a]}}(x) = \min_{a_s \in [a]} f(a_s,x)$ and $\overline{g_{[a]}}(x) = \max_{a_s \in [a]} f(a_s,x)$, and we show that these two functions are piecewise polynomial functions, with coefficients in $\{\overline{f_i([a])}, \underline{f_i([a])}\}$. For instance, if $g_{[a]}(x) = [-2,3]x^2 + [-4,-2]x + [4,5]$, then $\overline{g_{[a]}}(x) = g^+(x)$ for $x \geq 0$, and $\overline{g_{[a]}}(x) = g^-(x)$ for $x \leq 0$, with $g^+(x) = 3x^2 - 2x + 5$ and $g^-(x) = 3x^2 - 4x + 5$. The key point is to work with these two (univalued) functions $\underline{g_{[a]}}$ and $\overline{g_{[a]}}$ instead of $g_{[a]}$ (multivalued).

Let us describe the determination of l. The evaluation of $\overline{g_{[a]}}$ and $\underline{g_{[a]}}$ on $\underline{[x]}$ determines with which extremal function to work, e.g., with $\overline{g_{[a]}}$. According to the degree d of the polynomial, the roots of $\overline{g_{[a]}}(x) = 0$ are then determined either analytically ($d \leq 4$), or numerically ($d \geq 5$). For

$d \geq 5$, we use `BoxRevise` which converges quickly since it is applied to a univalued function.

This idea has been sketched in two pages by Van hentenryck et al. in [2] and implemented in the solver Numerica. We go beyond this raw idea, present in detail a new implementation of it and provide a full experimental evaluation of the approach that shows the efficiency of an algorithm based on extremal functions. `PolyBox` has been implemented in `Mathematica` and in the interval-based solver `Ibex` in `C++`.

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Keywords: Interval analysis, numerical CSPs, contraction, Box consistency, extremal functions

Using OpenMP to Parallelize Interval Algorithms

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Many interval applications exhibit a certain level of parallelism. Sometimes there is even more than one level.

The Message Passing Interface MPI [1] is a wide spread distributed memory programming model used to parallelize applications.

A program parallelized with MPI typically performs best if the parallelism is implemented at a fairly high level. For example, it may be hard to efficiently parallelize a loop that performs relatively simple computational operations only.

The learning curve for MPI is quite steep. It may also be less suitable in case the communication to computation ratio is high. In such situations, OpenMP [2], [3] could be an alternative.

OpenMP is a shared memory parallel programming model, available for over a decade and very suitable to implement parallelism in (interval) applications. Several important features make it an interesting option to consider. It also naturally maps onto the hardware parallelism available in multicore processors.

In some programs, a hybrid approach is even feasible. In such a case, MPI is used to implement a coarse grained level of parallelism, while OpenMP is applied to parallelize the finer grained part(s).

When parallelizing an (interval) application, good compiler support and tools are indispensable.

The Sun Studio Fortran and C++ compilers support interval arithmetic since 2000 [4,5]. In particular the Fortran implementation is very elegant. It uses a native "interval" data type. In C++, support for intervals is provided through a class library.

A profiler guides the developer what time consuming parts of the program have to be parallelized. Such a tool should also inform on performance bottlenecks in the parallel version of the program.

There is also the issue of correctness. Two of the most notorious problems in shared memory parallel programs are deadlock (or livelock), and data races. In case of the former, the threads do not make any progress, causing the application to hang.

A data race occurs if two or more threads access the same, and therefore shared, memory location, at least one of these accesses is a write operation on this region in memory, and there is no common lock to prevent simultaneous access.

The way a data race manifests itself is rather unpleasant. It leads to silent data corruption in memory, resulting in incorrect numerical results. Given there is a dependence on the relative execution of the threads, a data race may not even show up for a long time.

Intervals are by no means exempt from these problems and therefore tools in this area not only reduce the development time, but also increase the reliability of the application. For example, a data race may, or may not, result in a containment failure. Such a failure is however a lucky situation and is not guaranteed to occur.

In this paper[2] we give a short overview of the support provided for intervals in the Sun Studio Fortran compiler in particular. This is followed by a brief introduction into OpenMP.

Through a case study we then show how an example interval program is parallelized with OpenMP.

The Sun Performance Analyzer provides extensive profiling capabilities. We show how it is used to analyze the performance of an interval application.

The Sun Thread Analyzer detects deadlock and data races in a shared memory parallel program. Using the OpenMP example program we demonstrate how to detect a data race with this tool.

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[6] http://hpc.sun.com/page/articles

Keywords: Intervals, interval arithmetic, OpenMP, performance, correctness, deadlock, livelock, data race, Sun Studio

[2]The full version of this paper is available at [6].

Interval Methods for Inverting Operations and Solving Equations

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In the early days of interval analysis, the functional definition of division between intervals A and B was used:

$$A/B \stackrel{\text{def}}{=} \{x/y \mid x \in A \text{ and } y \in B\}.$$

The problem that this is not defined when $0 \in B$ was solved by Ratz's [5] *relational definition* of interval division: A/B defined as the smallest interval containing

$$\{z \in R \mid x = y * z \text{ and } x \in A \text{ and } y \in B\}.$$

Multiplication is an easy case: its inverse is at least a function, albeit a partial one. The binary operation max, where $max(x, y)$ is the greater of x and y, is more challenging: its inverse is multivalued. We show that in this case the relational definition yields a simple computation rule for the interval inverse of max between intervals:

$$\max^{-1}([c,d],[a,b]) = \begin{cases} \text{if } b < c\text{:} & \emptyset \\ \text{if } b \geq c \text{ and } a < d\text{:} & [-\infty, b] \\ \text{if } b \geq c \text{ and } a \geq d\text{:} & [a,b] \end{cases}$$

The relation used in the relational method need not be defined by a function, as it was in the case of multiplication and max. We next consider the relation $\leq$ and ask: For what intervals A and B should the relation $A \leq B$ be considered true? The answer obtained by the relational method sheds light on the controversial issue.

The relational method is not restricted to intervals. It applies equally well to relations over arbitrary sets, as well as of arbitrary arity. In this general case, the relational method suggest the definition, for a given n-ary relation r, the n *companion functions* for r. These functions are a convenient way of defining the *domain-reduction operation* for r, as found in constraint-solving [1,2].

Ratz's definition of interval division and the interval inverse of max are found to be simple applications of the domain-reduction operation. Domain-reduction operations open up further possibilities. Determining the inverse of multiplication can be viewed as solving the equation $ax - b = 0$ The solution of this equation with domain-reduction operations suggests using them for the solution of systems of m nonlinear equations in n unknowns. The algorithm we derive for solving such systems by means of domain-reduction operations is similar to SIVIA [3,4].

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Constraint-Driven Global Optimization

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We have developed a derivative-free algorithm for the verified determination of the location and level of the global optimum of a nonlinear objective function under nonlinear inequality constraints. Without loss of generality we consider the *minimization* formulation of the optimization problem.

For the unconstrained version of the problem there is the well-known Moore-Skelboe algorithm, which is a branch-and-bound search where effective cut-offs depend on tight upper bounds on the objective function. In the constrained version, however, we need verified feasibility of boxes to obtain any upper bound. This requirement makes Moore-Skelboe unsuitable as starting point.

The way ahead is to take constraint solving as starting point. From this point of view, the objective function becomes a preference criterion for selecting one among what is typically a continuum of solutions to the constraints. The feasible set defined by the inequality constraints may be empty. If it is not empty, then this set's interior (in the sense of topology) is typically also nonempty, but may be empty in degenerate cases.

We use as constraint solver SIVIA [1], an interval algorithm for the verified solution of systems of nonlinear inequalities with properties that make it suitable for our purpose. SIVIA yields two lists of boxes, I and B. The boxes in these lists are mutually non-overlapping. The union of the boxes in I is contained in the interior of the feasible set. The union of the boxes in B contains the boundary of the feasible set.

We adapt SIVIA in two stages. The first stage is to make it more effective as a constraint solver. The second stage is to incorporate certain features of Moore-Skelboe so that as much as possible only boxes are subdivided that may contain the constrained global minimum.

In the first stage, we transform SIVIA from its original recursive form to one that is controlled by a list U of boxes that cannot be placed in I or B. U is a priority queue ordered in such a way as to yield as quickly as possible a box in I.

In the second stage, I is also made into a priority queue, managed as it would be by Moore-Skelboe. The upper bounds thus found not only eliminate boxes from I, but also from U and B.

Our resulting algorithm for nonlinear global optimization with nonlinear inequality constraints has the following properties:

1. verified bounds for the level of the global minimum
2. verified box for the location of the global minimum
3. guaranteed termination
4. highly probable indication of whether the global optimum occurs at the boundary
5. for non-boundary optimum, the time and space requirements are asymptotically those of Moore-Skelboe

Our algorithm is an interval *arithmetic* algorithm. However the improvements demonstrated or claimed in the literature [2-5] obtainable by interval *constraints* are applicable to our algorithm as well.

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Estimating Variance under Interval Uncertainty: Parallel Algorithms

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Traditional data processing in science and engineering starts with computing the basic statistical characteristics such as the population mean E and population variance V. In computing these characteristics, it is usually assumed that the corresponding data values $x_1, \ldots, x_n$ are known exactly. In many practical situations, we only know intervals $[\underline{x}_i, \overline{x}_i]$ that contain the actual (unknown) values of x_i. In this case, different possible values of x_i lead, in general, to different values of E and V. In such situations, we are interested in producing the intervals of possible values of E and V – or fuzzy numbers describing E and V. There exist algorithms for producing such interval estimates; see, e.g., [1,2].

However, these algorithms are more complex than the typical data processing formulas and thus, require a larger amount of computation time. If we have several processors, then, it is desirable to perform these algorithms in parallel on several processors, and thus, to speed up computations. In this talk, we show how the algorithms for estimating variance under interval uncertainty can be parallelized.

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Keywords: statistics, interval uncertainty, parallelization

Filib++ and the Coming Interval Standard

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Filib++ is a well-known and frequently used C++ library for interval arithmetic. The design uses templates and traits classes to obtain an efficient, easily extendable, and portable C++ library.

Currently an interval is a template with 3 template parameters, one type parameter for the underlying base class and two flags, the first specifying the switch of rounding modes including simulation of the directed roundings, and the second specifying the so-called mode of interval evaluation, namely traditional interval mode with the strict evaluation of functions only if the argument interval is a subset of the domain of the function or containment mode preferring the loose evaluation. Because this loose evaluation of functions may cause problem when we implement algorithms that rely on the continuity of the function (Brouwer's fixpoint theorem, e.g.) a discontinuity flag has to be set. The handling of that flag in the environment of multi-threaded, multi-tasking, superscalar computer systems will be discussed, As base types usually all floating-point types may be used, as well as user defined types which provide their operations via an appropriate traits class. (A traits class is a template with adaptable information about its instantiating data type.)

Unfortunately the improvement of the optimization capabilities of compilers has led to the fact that some of the basic operations are written in assembler code. We investigate alternatives in this talk. One of the most powerful would be to have standard operations for intervals or at least for operations with directed rounding. By the time of this writing the initiative to include a definition of interval arithmetic into the revision of the IEEE standard 754 for floating-point arithmetic seems to have failed. A study group is working on a separate interval arithmetic standard. filib++ will have been extended to serve as a reference implementation for that standard, in particular there is an exact sum and inner product operation to support variable length interval arithmetic.

Keywords: interval arithmetic libraries

Estimating Maximal Information Amount under Interval Uncertainty

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In most practical situations, our knowledge is incomplete: we do not know the exact state s of the world, instead, there are multiple different states $s_1, \ldots, s_n$ which are consistent with our knowledge. In such situations, it is desirable to gauge this uncertainty, and a natural measure of uncertainty is the average number of binary ("yes"-"no") questions that we need to ask to find the exact state s.

According to Shannon's *information theory*, when we know the probabilities $p_1, \ldots, p_n$ of different states $s_1, \ldots, s_n$ respectively (for which $\sum_{i=1}^{n} p_i = 1$), then the above-described average number of binary questions is equal to $S = -\sum_{i=1}^{n} p_i \cdot \log_2(p_i)$. This average number of questions is called the *amount of information*.

In practice, we rarely know the exact values of the probabilities p_i. These probabilities are often only known with uncertainty. In many practical situations, we only know intervals

$$[\underline{x}_1, \overline{x}_1], \ldots, [\underline{x}_n, \overline{x}_n],$$

such that for each i from 1 to n, the probability $p_i = \dfrac{x_i}{\sum_{j=1}^{n} x_j}$, where $x_i \in [\underline{x}_i, \overline{x}_i]$. For different values $x_i \in [\underline{x}_i, \overline{x}_i]$, we get, in general, different values of p_i, and in turn, different values of the information amount S. To gauge the corresponding uncertainty, it is desirable to find the largest possible value of S, i.e, the maximal information amount $\overline{S}$.

Thus, we arrive at the following computational problem: given n intervals $[\underline{x}_1, \overline{x}_1], \ldots, [\underline{x}_n, \overline{x}_n]$, find the maximum $\overline{S}$ of the range

$$\mathbf{S} = \left\{ -\sum_{i=1}^{n} \left(\frac{x_i}{\sum_{j=1}^{n} x_j} \right) \cdot \log_2 \left(\frac{x_i}{\sum_{j=1}^{n} x_j} \right) \,|\, x_i \in [\underline{x}_i, \overline{x}_i] \right\}.$$

In [1], a polynomial algorithm for computing $\overline{S}$ has been presented for solving this problem. In this paper, we propose a new faster algorithm for computing $\overline{S}$ which only requires $O(n \cdot \log(n))$ time.

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LP Narrowing: A New Strategy for Finding All Solutions of Nonlinear Equations

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An efficient algorithm is proposed for finding all solutions of systems of n nonlinear equations using a new strategy called LP narrowing. In the LP narrowing strategy, boxes (n-dimensional rectangles in the solution domain) containing no solution are excluded, and boxes containing solutions are narrowed so that no solution is lost. Since the LP narrowing is very powerful, all solutions can be found very efficiently. By numerical examples, it is shown that the proposed algorithm could find all solutions of systems of $4000 \sim 50000$ nonlinear equations in practical computation time. Two numerical examples are shown in the next page.

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Keywords: Nonlinear equations, interval analysis, finding all solutions

Numerical Examples

Example 1 (known as Yamamura1 in the INRIA benchmark problems)

$$2.5x_i^3 - 10.5x_i^2 + 11.8x_i + \sum_{i=1}^{n} x_i - i = 0, \qquad i = 1, 2, \ldots, n$$

Example 2 (known as Bratu in the INRIA benchmark problems)

$$x_{i+1} - 2x_i + x_{i-1} + h^2 \exp(x_i) = 0, \qquad i = 1, 2, \ldots, n$$

where $x_0 = x_{n+1} = 0$ and $h = 1/(n+1)$

Table 1: Comparison of computation time (s) in Example 1.

n	S	Ref.[3]	Proposed
100	9	49	0.31
200	13	1 259	3
300	11	10 649	9
400	9	36 854	23
500	13	90 055	54
⋮	⋮	⋮	⋮
1000	17	∞	639
1500	13	∞	2 600
2000	9	∞	5 113
2500	9	∞	11 354
3000	27	∞	37 261
3500	15	∞	40 377
4000	21	∞	98 170

Table 2: Comparison of computation time (s) in Example 2.

n	S	Ref.[3]	Proposed
50	2	63	0.02
100	2	7 143	0.06
150	2	142 749	0.13
⋮	⋮	⋮	⋮
1000	2	∞	5
2000	2	∞	20
3000	2	∞	46
4000	2	∞	85
5000	2	∞	155
6000	2	∞	252
7000	2	∞	376
8000	2	∞	533
9000	2	∞	727
10000	2	∞	964
⋮	⋮	⋮	⋮
20000	2	∞	5 836
30000	2	∞	14 489
40000	2	∞	27 702
50000	2	∞	44 942

S: Number of solutions obtained by the algorithms

∞: It could not be computed in practical computation time

Computer: Dell Precision T7400 (CPU: Intel Xeon 3.4GHz)

Fast Verified Automatic Integration using Double Exponential Formula

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This talk is concerned with verified numerical integration of a univariable function with respect to x from -1 to 1. To verify the integrand, we propose a fast verified automatic integration algorithm. Automatic integration algorithm means that we input a problem and a tolerance for relative error, and it outputs an interval including the true value, whose diameter is smaller than the tolerance.

We adopt the double exponential formula as a quadrature in this research. The double exponential formula was proposed by H. Takahashi and M. Mori in 1974. It uses variable transformation $x = \phi(t)$ which transforms the original integral into $I = \int_{-\infty}^{\infty} f(\phi(t))\phi'(t)dt$, and after the transformation it uses the trapezoidal formula for I over $(-\infty, \infty)$. This formula is able to output a numerical solution with very high accuracy for the definite integral $I = \int_{-1}^{1} f(x)dx$, even if there are singular points on the edge of the integral interval. Its error is expressed as $\mathcal{O}(\exp(-CN/\log N))$ as a function of $N\,(= 2n + 1)$, which is the number of function evaluations. Since the integrand decays double exponentially after the transformation, it is called the double exponential formula.

A verified algorithm for the double exponential formula has been already proposed by Kobata [1]. In this talk, we improved this algorithm in two aspects: First we improve it with respect to the algorithm of computing n, which is the number of points of the double exponential formula and satisfies the tolerance. We propose new algorithm for getting smaller n than Kobata's one. In addition, we improve the algorithm by Kobata with respect to the algorithm of computing the upper bound of the rounding errors. Though we can use the interval arithmetic to know how much the rounding errors occur, it sometimes becomes much slower than pure floating-point arithmetic. To speed up the algorithm, we adopt an priori error evaluation method proposed by Kashiwagi [2], whose algorithm is to compute an upper bound of the maximum rounding error for function evaluation in every points of the integral interval. After running this algorithm once, we only need to execute pure floating-point arithmetic for the function evaluations, so that the proposed algorithm get much faster.

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Keywords: Integration, Verification, Double Exponential Formula

Enclosure of the Solutions to Interval Fredholm Equations of the First and Second Kind

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Integral equations often result from a weak form formulation when computing solutions to physical systems. There exist rare cases where exact solutions to integral equations can be computed, however, most of the solutions to integral equations are obtained approximately by numerical methods. Using conventional methods, the degree of accuracy of the numerical solution cannot be verified since in general the exact solution is unknown. The method presented in this paper obtains guaranteed enclosure of the solutions to Fredholm Equation of the First and Second Kind using the developed Interval Kernel Splitting Technique. The technique was used successfully by the authors [5] to obtain guaranteed bounds on the discretization error to boundary element method. The method is general and does not require any special property of the Fredholm Equations other than that the solutions are unique and finite over their domains. The uniqueness requirement allows for solvability and the finite solution requirement allows for obtaining meaningful enclosure and is not necessary for the guarantee of the enclosure. In this paper the technique is extended to obtain guaranteed enclosure to Fredholm Equation of the Second Kind with the same restrictions on the solutions. Standard numerical approximations of the solutions are used to obtain interval linear system of equations and a transformation of the resulting system to the standard interval linear system of equations is presented. The system is parameterized with respect to the location at which the approximate solution is calculated in order to achieve finite interval bounds. Parameterized Krawczyk iteration [3,4] is reviewed for clarity and further parameterization is utilized to improve the quality of the enclosure. Examples are presented for equations of both types to illustrate the method and its behavior with increasing number of domain subdivision.

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Keywords: Interval Fredholm Equation, Interval Enclosure

Fixed-Motion Shadowing on Gravitational n-Body Simulations

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We study the reliability of high-dimensional gravitational n-body simulations by using shadowing. A *shadow* of a numerical trajectory is an exact trajectory that stays close to the numerical one for a long time. The shadowing algorithm that we use here is essentially the refinement proceduce proposed in [2], generalized to high-dimensional systems by Quinland and Tremaine [5], optimized to be about 10^2 times faster by Hayes [3], and then modified to work on existing large simulations by the authors. In one iteration of refinement, we use accurate integrations to estimate the full phase-space errors at each timestep of the trajectory, and then iterate on Newton's method to drive those errors to zero; a trajectory with zero error is by definition exact, and if it lies close to the original, then it is by definition a shadow.

Astronomers perform simulations of up to $N = 10^9$ particles. Since shadowing takes $O(N^3)$ time, it is infeasible on such systems. However, we can shadow the trajectory of one particle at a time, moving in the gravitational potential of all the others. This is called "fixed-motion shadowing". Based on this idea, we fixed-motion shadow a 10^6-particle simulation of Dubinski [1], which simulates a collision of two galaxies. We investigate the dependency of shadow lengths on the number of particles N, the timestep h, and other physical parameters used by astronomers in their simulations.

Since the high precision integrator uses smaller time-steps to compute a more accurate trajectory, we use interpolation between two original time-steps to obtain a continuous trajectory of all the particles except the one being shadowed. We also use an exact (correctly rounded) summation of the forces, in comparison to the approximate force calculation done by astronomers. There are three kinds of particles in original Dubinski's simulation, designed to mimic three distinct populations of matter in real spiral galaxies: disk stars (which tend to be young), central bulge stars (which tend to be old), and halo (which is dark matter of unknown composition). We randomly pick 100 particles of each kind per galaxy to shadow. It takes about a week of CPU to find a shadow for one particle. The result is, halo particles have the longest average shadow length, lasting a substantial fraction of the duration of the simulation. The average shadow lengths of disk and bulge are much shorter, lasting only a small fraction of the full simulation time. The physical significance of these results is as yet unclear.

We also attempt shadowing of particles in one stable galaxy (that is, in the absence of the collision done by Dubinski [1]) and find that the shadows last longer. Furthermore, the shadow lengths better fit an hypothesis published by Hayes [4]. This result shows that the formula works best for bulge, and not too bad for disk and halo. We will present some explanations for this phenomenon. Our ultimate goal is to help astronomers do n-body simulations with appropriate time-step values and softening lengths, which have long average shadow lengths.

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Efficient Parallel Solvers for Large Dense Systems of Linear Interval Equations

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We present newly developed self-verifying parallel linear system solvers based on MPI. These solvers use BLACS, ScaLAPACK and fast algorithms for dot products in (simulated) higher precision using so called error free transformations [1]. By using these methods and the possibilities of the C-XSC library [2], the solvers are fast but achieve a high accuracy compared to other solvers. Furthermore, by distributing the required data equally among all nodes used in the parallel computations, it is possible to compute a verified solution of very large systems with dense system matrices using a cluster computer with sufficient memory resources per node (in our testing we were able to compute a verified solution of a real dense linear point system of dimension 100000×100000). We discuss the expected numerical quality of the new solvers and we compare their speed, memory consumption and scalability to more traditional solvers. Detailed time analysis will be given for different parallel computing platforms to show further challenges for the improvement of our algorithms.

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