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A B S T R A C T S

Stochastic Arithmetic, Theory and Experiments

René Alt*, Jean-Luc Lamotte*, Svetoslav Markov**

*Laboratory LIP6
University Pierre et Marie Curie – Paris 6, France
Rene.Alt@lip6.fr, Jean-Luc.Lamotte@lip6.fr

**Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
smarkov@bio.bas.bg

Stochastic arithmetic is an old idea [8] and has been first formalized by J. Vignes and J. M. Chesneaux [5], [9]. In fact stochastic arithmetic is a model for computing with unprecise data when they belong to some known gaussian distribution $N(\mu,\ \sigma)$. These unprecise data are called stochastic numbers and the computation on them is called stochastic arithmetic which is merely operations on gaussian distributions. In this sense, stochastic arithmetic provides a confidence interval for the result of numerical computation in the same way that interval arithmetic provides exact bounds for this result. It must also be remarked that the operations of stochastic arithmetic resemble the same operations for intervals when they are written in the center radius form. Moreover, stochastic arithmetic is also a model for the random rounding arithmetic which is implemented in the Cestac method and the Cadna Software [9]–[10]. Many of the properties of stochastic arithmetic and stochastic numbers have been studied from the point of view of abstract algebraic structures, see [1]–[3], [6]–[7]. In particular it has been shown that stochastic numbers have a structure called S-space which is very close to vector space. Some experiments have also been done to illustrate the theory. For example it has been shown in [4] that the confidence interval of the result of an inner product of two n-dimensional vectors, one with exact data and the other with imprecise data increases proportionally to $\sqrt{n}$ and consequently in some condition, the accuracy may increase with the dimension. Here in the same direction, the authors have proved that this property is also true for two vectors with imprecise data. A theoretical formula is given for the error on the result. Moreover an experimental software has been developed which implements stochastic arithmetic. This software allows very easily to run a standard code written in Fortran or in C++ with stochastic arithmetic. Some classical experiments such as computing inner products, solving linear systems, solving polynomials, always with unprecise data are reported. In each case a confidence interval for the solution (or for the components of the solution) is provided. The obtained results conform to the theory and show that a straightforward use of stochastic arithmetic may easily lead to instructive features of a numerical problem such as the detection of instabilities.

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Parameter Identification of a Fed-batch Cultivation of *S. cerevisiae* Using Genetic Algorithms

Maria Angelova, Tania Pencheva, Stoyan Tzonkov
Centre of Biomedical Engineering
Bulgarian Academy of Sciences
maria@clbme.bas.bg, tania.pencheva@clbme.bas.bg,
tzonkov@clbme.bas.bg

Fermentation processes as objects of modelling and high-quality control are characterized with interdependence and time-varying of process variables that lead to non-linear models with a very complex structure. That is why the conventional optimization methods can not lead to a satisfied solution. As an alternative, genetic algorithms, like stochastic global optimization method, can be applied to overcome these limitations. The application of genetic algorithms is a precondition for robustness and reaching of global minimum that makes them eligible and more workable for parameter identification of fermentation models. Different types of genetic algorithms, namely simple, modified and multi-population ones, have been applied and compared for estimation of nonlinear dynamic model parameters of fed-batch cultivation of *S. cerevisiae*.

Efficient Generation of the Scrambled Halton Sequence Using Specific Optimizations

Emanouil Atanassov, Mariya Durchova
Institute for Parallel Processing
Bulgarian Academy of Sciences
mabs@parallel.bas.bg

The Halton sequence is one of the first and popular low-discrepancy sequences. Various modifications of the original construction of Halton are developed and studied. These modifications usually provide significant improvement in the convergence rate of the resulting quasi-Monte Carlo algorithms. One of the most promising types of modification is the scrambling, described by Owen. Since the base of the number systems that are used, is different for every coordinate, the implementation of this technique faces technical difficulties and can be unfeasible for many important applications. Instead of original Owen's scrambling, in this paper we describe implementation of a simplified scrambling technique (linear

permutations) which utilizes specific hardware in order to achieve better speed of generation. We describe the algorithm in detail and provide timing results demonstrating the applicability of the approach for Grid applications.

GPU-based Generation of Scrambled Sobol Sequence

Emanouil Atanassov, Aneta Karaivanova, Sofiya Ivanovska
Institute for Parallel Processing
Bulgarian Academy of Sciences
sofia@parallel.bas.bg

Sobol sequence is the most widely used low discrepancy sequence for numerical solving of multiple integrals and other quasi-Monte Carlo computations. Owen first proposed scrambling of this sequence through permutation in a manner that maintained its low discrepancy. Scrambling is necessary not only for error analysis but for parallel implementations. Good scrambling is especially important for GRID applications. However, scrambling is often difficult to implement and time consuming. In this paper we propose fast generation of Sobol sequence with Owen scrambling, using GPU computing. Numerical and timing results, demonstrating the advantages of our approach are presented and discussed. In addition, numerical and timing results for solving multidimensional integrals (up to 100-dimension) using GPU-based scrambled Sobol sequence generation are presented and compared to other approaches.

Mathematical Modeling for Studying Microbial Processes – Some Examples

Venko Beschkov, T. Sapundzhiev, K. Petrov, E. Vasileva
Institute of Chemical Engineering
Bulgarian Academy of Sciences
bioreac@bas.bg

Mathematical modeling may have different purposes in chemical and biochemical engineering sciences. One of them is to confirm or to reject kinetic models for certain processes, or to evaluate the importance of some transport phenomena on the net chemical or biochemical reaction rate. In the present paper different

microbial processes are considered and modeled for evaluation of kinetic constants for batch and continuous processes accomplished by free and immobilized microbial cells. The practical examples are from the field of wastewater treatment and biosynthesis of products, like enzymes, lactic acid, gluconic acid, etc. By the aid of the mathematical modeling the kinetics and the type of inhibition is specified for microbial wastewater denitrification and biodegradation of halogenated hydrocarbons. The importance of free and immobilized cells and their separate contribution to the overall microbial process is also evaluated for some fermentation processes: gluconic acid production, dichloroethane biodegradation, lactic acid fermentation, etc.

Extension of the C-XSC Library with Scalar Products with Selectable Precision

Gerd Bohlender*, Werner Hofschuster**, Walter Krämer**, Michael Zimmer**

*University of Karlsruhe, Germany

bohlender@math.uka.de

**University of Wuppertal, Germany

kraemer@math.uni-wuppertal.de

The C++ class library C-XSC for scientific computing has been extended in version 2.3.0 by scalar products with selectable precision. This is in contrast with prior versions which always computed scalar products exactly with the help of the so-called long accumulator. This article gives a detailed description of the algorithms used and of their implementation as well as some hints on potential pitfalls which may occur in compilation. Furthermore, we also briefly explain the theoretical background of the DotK algorithm and the necessary modifications in the concrete implementation in C-XSC. Runtime tests and numerical examples are also given.

Note: the significantly improved runtime behaviour of C-XSC by means of the so-called DotK algorithms is only due to the unfortunate fact that the long accumulator is still not supported in hardware on present processors. Such a hardware support has been frequently requested. It would guarantee scalar products of floating-point vectors to be always exact and to have optimal performance (i. e. much faster than with all known DotK algorithms – even with possible hardware support).

A Mathematical Basis for an Interval Arithmetic Standard

Gerd Bohlender, Ulrich Kulisch
University of Karlsruhe, Germany
bohlender@math.uka.de, kulisch@math.uka.de

The IEEE Interval Standard Working Group P1788 is working on a future standard for interval arithmetic. We present the current status of the discussions and propose a mathematical basis for the definition of interval arithmetic operations.

Interval arithmetic deals with closed and connected sets of real numbers. It is free of exceptions. A complete set of formulas to approximate real interval arithmetic on the computer is displayed in this paper. The essential comparison relations and lattice operations are also discussed. Evaluation of functions for interval arguments is studied. The requirement to adapt the digital computer to the needs of interval arithmetic is as old as interval arithmetic itself; a simple possible solution is presented. The desirability of variable length interval arithmetic is also discussed in the paper.

One-Parameter Bifurcation Analysis of Dynamical Systems Using MAPLE

Milen Borisov, Neli Dimitrova
Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
milen_kb@abv.bg, nelid@bio.bas.bg

Biotechnological processes are modelled by systems of autonomous ordinary differential equations depending on parameters. Given such a system, the ultimate goal is to obtain its bifurcation diagram, that is to divide the parameter space into regions within which the system has topologically equivalent phase portraits. The center manifold theory proposes a systematic way for simplifying dynamical systems. Reducing a dynamic system to its center manifold means computation of a parameter-dependent normal form for each bifurcation in the minimal possible phase space dimension and specification of the relevant genericity conditions. The parameter and coordinate transformations required to put the system into the normal form lead to lengthy intermediate calculations and expressions. The natural environment for such kind of work are the computer algebra systems. Their impact on dynamical systems studies is due to the fact that many calculations are too tedious for manual work but do not challenge the computer resources.

In this paper we propose algorithms and procedures in *Maple* for symbolic reduction of the dynamic system to the center manifold related with the one-parameter local bifurcations of fixed points. The procedures are applied to investigation of models of biological processes.

Model-Based Biological Control of the Chemostat: New Results and Applications

Neli Dimitrova
Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
nelid@bio.bas.bg

The competitive exclusion principle (CEP) is a well known concept in microbial ecology. CEP means that when two or more microbial species grow on a single resource in a chemostat, at most one species eventually survives – this is the species that possesses the best affinity to the substrate.

CEP has been proved for models of the chemostat involving different response functions (like Monod and Haldane laws) and different population-specific removal rates.

Based on CEP, the original concept of the so called biological control of the chemostat has been recently developed (Rapaport and Harmand, 2008). The main idea consisits in adding particular species in the chemostat to globally stabilize an unstable biological process.

In this paper we present a generalization of the above mentioned result and apply it to a practical problem.

On the Ill-Posedness of Observation Problems

S. Diop
Laboratoire des Signaux & Systèmes
Supélec, France
diop@lss.supelec.fr

We call observation problems the estimation of state variables (or more generally, internal variables) from two sources of information: online measurements of some variables and the dynamic model relating the quantities to be estimated and the measurements. In the control theory engineering literature the tremendous

success of the Kalman filter has left little room to numerical analysis approaches to observation problems. This work is a contribution to the building of a tunnel between numerical analysis and engineering literature on observation problems. The first brick is seen to be the statement that state estimation is an ill-posed inverse problem. This is the aim of the present communication. More precisely, we restrict ourselves to linear systems (not necessarily with constant coefficients).

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Generalized Modelling: Turning Diagrams into Dynamics

Thilo Gross

Max-Planck Institute for the Physics of Complex Systems
Dresden, Germany

gross@pks.mpg.de

One of the central challenges of theoretical biology is to extract the dynamics from a given diagramatic representation of a biological system, based on limited information. This challenge is addressed by generalized modelling. Instead of restricting all functions in a system of differential equations to specific functional forms, we leave some or all of these functions unspecified. A generalized model can thus represent all plausible models consistent with given diagram. In the generalized model one can then identify the properties of the unknown functions that

one needed to know in order to determine the stability of arbitrary steady states in the system. This information can be captured by a number of unknown, but well-defined and well interpretable parameters. In this way we obtain a direct parameterization of the Jacobian describing the dynamics close to every steady state in every model that is consistent with the given diagram. While the exploration of the Jacobian reveals only limited information, it does so with a high degree and generality. This will be illustrated by several examples.

Quasi-Monte Carlo Algorithms for Matrix Computations

Aneta Karaivanova
Institute for Parallel Processing
Bulgarian Academy of Sciences
anet@parallel.bas.bg

The first application of Monte Carlo Methods (MCMs) in linear algebra appeared in a paper by Forsythe and Leibler in 1950. In the following years significant contributions were made, especially by Wasow, Curtiss, Halton, Hammersley and Handscomb and Sobol. These methods were recognizes as useful when obtaining a quick rough estimate of solution, when the problem is too large or too intricate for any other treatment, or when just one component of the solution vector or one element of the inverse matrix is desired.

There has been renewed interest in MCMs in recent times, the primary reason for this is the efficiency of parallel MCMs in the presence of high communication costs. The second reason for the recent interest in MCMs is that the methods have evolved significantly since the early days. Much of the effort in the development of Monte Carlo methods has been in the construction of variance reduction techniques which speed up the computation by reducing the rate of convergence of crude MCM, which is $O(N^{-1/2})$. An alternative approach to acceleration is to change the type of random sequence, and hence improve the behaviour with N. Quasi-Monte Carlo methods (QMCMs) use quasirandom (also known as low-discrepancy) sequences instead of pseudorandom sequences, with the resulting convergence rate for numerical integration being as good as $O((\log\ N)^k N^{-1})$. The first results of using QMCMs for linear algebra problems were presented by Mascagni and Karaivanova.

In this paper the convergence and the complexity of QMCMs for estimating the solution of systems of linear algebraic equations, inverting of matrices and finding extremal eigenvalues are studies. Numerical experiments with test sparse matrices are performed using different quasirandom number (QRN) sequences.

The results indicate that for all of the considered problems improvements in both the magnitude of the error and the convergence rate can be achieved using QRNs in place of pseudorandom numbers.

High-Order Control Variations and Small-time Local Controllability

Mikhail I. Krastanov
Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
krast@math.bas.bg

A basic idea of the so called geometrical approach is to construct "control variations". Heuristically, if one can construct control variations in all possible directions, then the considered control system is small-time locally controllable.

Some concepts of control variations of higher order will be presented. The relation between these variations and some sufficient controllability results will be discussed. Special attention will be paid on the gap between the existing sufficient and necessary controllability conditions. Some illustrative examples will also be presented.

Computer-Assisted Proofs and Symbolic Computations

Walter Krämer
Department of Mathematics and Computer Science
University of Wuppertal, Germany
kraemer@math.uni-wuppertal.de

We discuss some main points of computer-assisted proofs based on reliable numerical computations. Such so called self-validated numerical methods in combination with exact symbolic manipulations result in very powerful mathematical software tools. These tools allow to prove mathematical statements (existence of a fixed point, of a solution of an ODE, of a zero of a continuous function, of a global minimum within a given range, etc.) using a digital computer. To validate the assertions of the underlying theorems fast finite precision arithmetic is used. The results are absolutely rigorous.

To demonstrate the power of reliable symbolic-numeric computations and to show how important appropriate data structures are with respect to their efficiency we investigate several tasks concerning dynamical systems.

New Architectures for Scientific Computing: Performance and Constraints

Jean-Luc Lamotte
Laboratory LIP6, University Pierre et Marie Curie – Paris 6, France
http://pequan.lip6.fr/~lamotte

Over the last 5 years, new architectures have been proposed for numerical computation: multicore, GPU, CELL, etc. All they have a very high level of performance if we count the number of possible operations performed per second. But the peak performances are reachable only for a sub-set of applications. The goal of this talk is to make an overview of the relation between the new architecture and the algorithms with a high performance point of view. The talk is organized into three parts. Firstly, the main architecture used for numerical computing will be presented: multicore processor, GPU and CELL processor. Secondly, the constraint of the memory access will be detailed and the consequence on applications will be explained. The notion of memory bandwidth applications and computing bound applications will be introduced. In the last part, an example on a part of the N-Body problem will be detailed on the CELL processor.

Maximum Clique and Similarity Measures

N. Malod-Dognin*, R. Andonov*, Nikola Yanev**
*INRIA Rennes – Bretagne Atlantique and University of Rennes 1, France
(nmaloddg,randonov)@irisa.fr
**University of Sofia and
Institute of Mathematics and Informatics, Bulgarian Academy of Sciences
choby@math.bas.bg

Motivation. A fruitful assumption in molecular biology is that proteins sharing close three-dimensional (3D) structures are likely to share a common function and in most cases derive from a same ancestor. Computing the similarity between two protein structures is therefore a crucial task and has been extensively investigated. Evaluating the similarity of two proteins can be done by finding an optimal one-to-one matching between their components, which is equivalent to identifying a

maximum weighted/unweighted clique in a specific k-partite graphs, also called "alignment graph". The idea of using cliques for resolving similarity is implemented in VAST (Vector Alignment Search Tool) – a software for aligning protein 3D structures largely used in NCBI (National Center for Biotechnology Information). The original VAST clique solver uses the well known Bron and Kerbosh algorithm (BK) whose efficiency appeals for improvement.

Results. We designed a dedicated algorithm for solving the maximum cardinality clique problem in k-partite graphs. Our computational results on real protein alignment instances show that our algorithm is much much faster not only than BK but even than the Östergård algorithm, which is one of the fastest clique finder. This stimulated us to suggest a novel counterpart of the Contact Map Overlap, recently proven to be efficient for evaluating protein similarity.

Simulation of Real Communication Systems

Nikolai L. Manev
Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
nlmanev@math.bas.bg

A Software package for simulation of communications through a noisy channel using coded M-QAM and M-PSK modulation is developed. Various encoding schemes and codes over residue rings are tested. The error performance of these schemes is compared with error performance of trellis coded modulation and with coded modulation scheme based on Gaussian integers.

A New Approach to Fuzzy Arithmetic

Antony Popov
Faculty of Mathematics and Informatics
Sofia University, Bulgaria
atpopov@fmi.uni-sofia.bg

Interval computations are computations using intervals with the aim to guarantee the result in particular in the presence of data uncertainties and rounding errors. Since the alpha-cuts of the fuzzy numbers are closed intervals, then the interval calculus is essential part of the computations with fuzzy numbers. A fuzzy number is a fuzzy subset of the real line, i. e. it represents a generalization of a real number like a function defined on the real line taking values in [0,1].

Any fuzzy number A satisfies the following conditions:

– its support is bounded;
– there exists only one x such that $A(x) = 1$;
– the alpha-cuts of A are closed intervals.

Mathematical morphology appeared first as a nonlinear efficient image processing tool, but after it was set on the basis of the theory of complete lattices a vast majority of applications have been developped. There are several approaches for fuzzifying mathematical morphology. In our work we step on the framework of Deng and Heijmans based on adjoint fuzzy logical operators – conjunctors and implicators. We generalize this definition presenting a universal framework. In a previous work it has been showed that there exists a close relation between interval and crisp morphological operations – binary dilations and erosions. Having in mind this relation and our general definition of fuzzy morphological operations, we can express the known arithmetic operations between fuzzy numbers through morphological ones and thus we can define inner operations between fuzzy numbers by analog to those between intervals defined by S. Markov. Namely, it becomes possible to define inner addition and multiplication of fuzzy numbers.

Possible applications in constructing pairwise alignment of protein sequence and microbial biomass development are discussed.

Two Approaches to Linear Systems Involving Complex Interval Parameters

Evgenija Popova*, Lubomir Kolev**, Walter Krämer***
*Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
epopova@bio.bas.bg
**Technical University, Sofia, Bulgaria
kolev.l@mail.bg
***University of Wuppertal, Germany
kraemer@math.uni-wuppertal.de

We consider linear systems whose data depend affine-linearly on uncertain parameters varying within complex intervals. Such systems are usual in the analysis of electrical circuits. The methodology for an efficient worst-case analysis of electrical circuits is important but is not sufficiently developed. We present an original research which compares two approaches for bounding the exact hull of the solution set to the above mentioned linear parametric systems.

The first approach is based on transforming the original n-dimensional system involving affine-linear dependencies between k-parameters varying within complex intervals into an equivalent $2n$-dimensional system involving rational dependencies between $2k$-parameters varying within real intervals. We do an advanced

computer-assisted proof (in the environment of *Mathematica*®) for the monotonic dependence of the parametric solution of the new system on the interval parameters and thus we are able to compute rigorous guaranteed bounds for the exact hull of the sought solution set.

The second approach presents a first time application of the parametric fixed-point iteration to linear systems whose data depend affine-linearly on complex interval parameters. To this end, we use the complex arithmetic in *Mathematica*® and *MathLink* connection to a newly developed C-XSC module for solving complex parametric linear systems.

We present the methodology and the software tools necessary for the application of both approaches, and discuss their pros and cons on the results for a sample electrical circuit model.

Stability Analysis of Some Nonlinear Anaerobic Digestion Models

Ivan Simeonov, Boyko Kalchev
Institute of Microbiology "St. Angeloff"
Bulgarian Academy of Sciences
issim@microbio.bas.bg

Anaerobic digestion (AD) is an effective biotechnological process for treating different agricultural, municipal and industrial wastes. However, it is a very unstable process in regard to the biogas reactor operation. This is due to the complicated interactions between different microbial species as well as to the complex transformations of the organic matter affected by a variety of environmental factors. In this context, the use of mathematical models is a powerful tool for investigations, optimization and control of the AD. Depending on the aim of the modelling, a large number of modelling approaches is available: mass balance models, black box models, heuristic models. The widest spread for AD processes have received dynamic models based on mass balances, and especially such of them, which are created for continuously stirred tank reactor (CSTR) mode. They consist of sets of non-linear ordinary differential equations and describe more accurately all microbiological and biochemical phenomena during the AD processes. The paper deals with stability analysis of some mass balance models of the AD in CSTR. The equilibrium states for some AD models have been obtained, solving sets of nonlinear algebraic equations, using Symbolic toolbox of Matlab. Their stability has been analyzed using the Lyapunov's first method. Some open problems concerning their global stability have been formulated.