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Numerical Computations: Theory and Algorithms

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Yaroslav D. Sergeyev

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Table of Contents

Numerical Computations: Theory and Algorithms International Conference and Summer School

17–23 June 2013, Falerna (CZ), Tyrrhenian Sea, Italy

Dear Participants,

Welcome to the International Conference and Summer School *NUMTA-2013* "Numerical Computations: Theory and Algorithms". The Conference is organized jointly by the University of Calabria, Department of Computer Engineering, Modeling, Electronics and Systems Science, Italy, and by the N. I. Lobachevsky State University of Nizhni Novgorod, Russia. The two universities have a 20 years long collaboration in the framework of the international research and educational program "Italian-Russian University" and this Conference is one of the major events prepared jointly by the two partner institutions. We are proud to inform you that NUMTA-2013 is organized by the partners in cooperation with the Society for Industrial and Applied Mathematics (SIAM), USA.

The goal of the Conference is to create a multidisciplinary round table for an open discussion on numerical modeling nature by using traditional and emerging computational paradigms. The Conference will discuss all aspects of numerical computations and modeling from foundations and philosophy to advanced numerical techniques. New technological challenges and fundamental ideas from theoretical computer science, linguistic, logic, set theory, and philosophy will meet requirements and new fresh applications from physics, chemistry, biology, and economy.

Researchers from both theoretical and applied sciences have been invited to use this excellent possibility to exchange ideas with leading scientists from different research fields. Papers discussing new computational paradigms, relations with foundations of mathematics, and their impact on natural sciences have been particularly solicited. A special attention during the Conference will be dedicated to numerical optimization techniques and a variety of issues related to theory and practice of the usage of infinities and infinitesimals in numerical computations. In particular, there will be a substantial bunch of talks dedicated to a new promising methodology allowing one to execute numerical computations with finite, infinite, and infinitesimal numbers on a new type of a computational device – the Infinity Computer patented in EU, Russia, and USA.

We are happy to inform you that researchers from the following 27 countries participate at the Conference: Argentina, Australia, Brazil, Canada, China, Egypt, Finland, France, Germany, Greece, India, Israel, Italy, Japan, Lithuania, New Zealand, Norway, Philippines, Russia, Saudi Arabia, South Africa, Spain, Sweden, Turkey, Ukraine, United Kingdom, and USA.

Authors of selected talks will be invited to submit full papers to two special issues dedicated to the Conference that will be published by the following prestigious international journals ran by Elsevier: *Applied Mathematics and Computation* and *Communications in Nonlinear Science and Numerical Simulation*.

The Organizing Committee thanks sponsors of the Conference for their support. Without their help this event would not happen:

- University of Calabria (Italy);
- N. I. Lobachevsky State University of Nizhni Novgorod (Russia);
- Department of Computer Engineering, Modeling, Electronics and Systems Science of the University of Calabria (Italy);
- Italian National Group for Scientific Computation of the National Institute for Advanced Mathematics "F. Severi";
- Institute of High Performance Computing and Networking of the National Research Council (Italy);
- International Association "Friends of the University of Calabria" (Italy).

We wish to all participants a very successful work and hope that the Conference will give you a lot of inspiration leading to new important results in your research.

Yaroslav D. Sergeyev
Distinguished Professor
Chairman of NUMTA-2013

Tutorials and Plenary Lectures

Computing with Patterns: Chemical Waves, Slime Mould and Crystals

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Keywords. Unconventional computing; reaction-diffusion; pattern formation.

Living systems show numerous, often unconventional, ways of information processing, which are adopted, exploited, mimicked in computer software and engineering devices. Research in nature-inspired computing aims to uncover novel principles of efficient information processing and computation in biological systems to develop novel, and potentially more efficient, non-standard algorithms and computing architectures, and also to implement conventional algorithms in non-silicon, or wet, substrates. Despite the profound potential offered by unconventional computing, only a handful of experimental prototypes are reported so far, for example gas-discharge analog path finder; maze-solving micro-fluidic circuits; geometrically constrained chemical computers; chemical reaction–diffusion processors; maze-solving chemo-tactic droplets; enzyme-based logical circuits; spatially extended crystallization computers for optimization and computational geometry; molecular logical gates and circuits [1,2]. In my talk I will discuss three families of growing pattern based computing devices: reaction-diffusion computers, crystallisation-based computers and slime mould computers. I will demonstrate how classical tasks of computational geometry and optimisation (Voronoi diagram, Delaunay triangulation, spanning trees, relative neighbourhood graphs, β-skeletons) can be approximated by excitation (Belousov-Zhabotinsky medium), crystallisation in supersaturated solutions or biological growth patterns (P. polycephalum) propagating in a quasi two-dimensional space and interacting with each other. I will explain how Boolean logical circuits can be implemented using collision-based computing paradigm executed in simulated and experimental laboratory non-linear media computers; and, present experimental designs of binary adders implemented in excitable chemical medium and slime mould.

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Recent Advances in Geometric Integration

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Keywords. Hamiltonian problems; geometric integration; energy-preserving methods.

We provide a self-contained introduction to *discrete line integral methods*, a class of energy-conserving Runge-Kutta methods recently devised for the numerical solution of Hamiltonian problems [1]. The basic idea on which the methods rely on will be fully discussed, along with a corresponding novel framework for the analysis of the methods [2].

The class of energy-conserving Runge-Kutta methods named HBVMs (*Hamiltonian Boundary Value Methods*) will be studied in detail [3], including the efficient solution of the generated discrete problems.

The same basic approach, based on a discretized line integral, is then extended to derive more general classes of methods, able to cope with *general* conservative problems, possibly having multiple invariants [4].

Further generalizations will be also sketched, along with future directions of investigation.

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The Use of Grossone in Mathematical Programming

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Keywords. Mathematical programming; simplex method; anticycling method; data envelopment analysis; nonlinear programming.

In this talk we will discuss some applications of ① in Mathematical Programming. The aim is to show how the use of the new methodology that has been proposed by Sergeyev for performing calculations with infinite and infinitesimal quantities could improve the efficiency of standard methods in nonlinear programming and will also clarify the role of penalty terms.

In particular, we will focus the attention on how new numeral system allows to define new differentiable penalty functions. Moreover, we will investigate the relationship between stationary points of this penalty function and KKT points for the original Nonlinear Programming problem.

Another application of ① that will be presented is related to the Data Envelopment Analysis (DEA) methodology, for evaluating the efficiency of Decision Making Units(DMU). The use of negative power of ① allows to define new linear programming problems with theoretical properties similar to those obtained using infinitesimal non–archimedean quantities.

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Canonical Duality and Triality: Unified Understanding Complex Systems and NP-hard Problems

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Keywords. Global optimization; NP-hard problems; canonical duality.

Canonical duality is a potentially powerful theory, which can be used to model complex phenomena within a unified framework. The associated triality theory reveals an interesting multi-scale duality pattern in complex systems, which can be used to identify both global and local extrema and to design efficient algorithms for solving a wide class of challenging problems in global optimization and computational science.

Beginning with some fundamental principles and basic concepts in mathematical physics, the speaker will show how the canonical duality theory be naturally and correctly developed and why a unified solution form can be obtained for totally different problems in nonconvex/discrete systems. Then he will explain the common misunderstandings on this theory, what is the open problem left in triality theory, and how this open problem is solved. Based on this canonical duality/trialtiy theory, he will first show how the NP-complete quadratic integer programming problem can be identically reformed as a continuous unconstrained Lipschitzian global optimization problem such that it can be solved via deterministic methods, then he explain the fundamental reason that leads to challenging problems in different fields, including NP-hard problems in global optimization and the paradox of Buridan's donkey in decision sciences. By using nonlinear perturbation methods in physics, he will present a new powerful primal-dual algorithm for solving general challenging problems in global optimization. Applications will be illustrated by certain well-known NP-Hard problems. He will show that in complex systems, the global minimizer may not be the best solution. Finally, some open problems and challenges will be addressed.

This talk should bring some fundamentally new insights into complex systems theory, global optimization and computational science.

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Tractable Minmaxmin Problems

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Keywords. Minmax; nonsmooth optimization.

Minmax optimization is of great importance for many real life applications as it is the election tool for dealing with decision making problems where the performance measure of any observed system is related to its worst-case behavior. Solving minmax optimization problems requires to deal explicitly with nonsmoothness of the objective function and, in some sense, the research in nonsmooth (or, equivalently, nondifferentiable) optimization has been strongly motivated by the need of tackling such family of problems.

The *minmaxmin* paradigm is a significant development of the *minmax* decision making approach; it is particularly suited for applications where both strategic and tactical decisions are to be made, at different points of time, in presence of uncertain scenarios.

The aim of the talk is to discuss some classes of minmaxmin problems, whose structure is well suited to represent some challenging real-life problems, and at the same time allows application of rather standard optimization techniques. The main contribution of the talk is in the treatment of a special class of minmaxmin problems, the bilinear minmaxmin problem, which reduces to solving a minmax problem where the max is taken over a finite set of concave, not necessarily differentiable functions. For such problems we provide an optimization scheme which is derived from standard approaches of nonsmooth optimization (bundle and conjugate subgradient methods) and exploits concavity of the component functions. We prove convergence of our method to a local minimum, and in addition we introduce a heuristic strategy for escaping from local minima. We report finally the results of some numerical experiments.

Parametric Global Optimization: Application to Sailboat Robotics

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Keywords. Interval analysis; sailboat robotics; non-convex optimization.

Introduction

A robot can generally be described by a vector first-order differential equation, named state equations. A robot is said to be redundant if it has more actuators than necessary. In this case, the number of inputs is higher than the number of outputs (variables to be controlled) and there exists many different ways to achieve the control requirements. We can thus take advantage of the extra number of freedom degrees in order to optimize some performance criterion (involving energy, security, longevity or speed). The resulting problem can be formalized into an parametric optimization problem with equality constraints where the free variables (or the parameters) of the optimization problem correspond to the outputs. Due the non-convexity of the optimization problem, the paper proposes to use an interval approach for the resolution. The approach is illustrated on the optimal sail tuning of a sailboat robot.

Formalism

Consider a mobile robot described by the following state equations

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}) \\ \mathbf{y} = \mathbf{g}(\mathbf{x}) \end{cases}$$

where $\mathbf{u} \in \mathbb{R}^m$ is the vector of inputs (or actuators) and $\mathbf{x} \in \mathbb{R}^n$ the state vector. The vector $\mathbf{y} \in \mathbb{R}^p$ is the vector of variables we want to control accurately. If $m > p$ the robot is overactuated and we will have different way to solve the control problem. In such a case, we may take advantage of this redundancies by maximizing a performance criterion $h(\mathbf{x})$. This criterion may correspond to the power delivered by the batteries (that we want to minimize) or to the speed of a boat (to be maximized), ... The corresponding optimization problem we have to solve is defined by

$$\hat{h}(\bar{\mathbf{y}}) = \max_{\bar{\mathbf{u}} \in \mathbb{R}^m, \bar{\mathbf{x}} \in \mathbb{R}^n} h(\bar{\mathbf{x}}) \qquad \text{s.t.} \begin{cases} \mathbf{0} = \mathbf{f}(\bar{\mathbf{x}}, \bar{\mathbf{u}}) \\ \bar{\mathbf{y}} = \mathbf{g}(\bar{\mathbf{x}}) \,. \end{cases}$$

The New Life of the Principle of Linguistic Relativity

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Keywords. Principle of linguistic relativity; Sapir–Whorf hypothesis; cognitive abilities; language and thought.

The principle of linguistic relativity (also known as the Sapir–Whorf hypothesis) has been actively discussed in the middle of the XX century. In its strong version it stated that language determines methods of cognition and thought of the speaker. Nowadays ideas about the relationship of language and thinking is becoming more and more popular (L. Boroditsky, S. Levinson, etc.).

Current research tends to go in two directions: attracting the material of rare languages and conducting experiments designed to compare cognitive abilities of speakers of different languages. Those experiments focus mostly on the solution of specific problems, in particular the spatial orientation.

Of particular value for modern approaches are languages that describe certain semantic and conceptual categories in a different from European way. The best known of these "exotic" languages is Pirahã. This language of Brazil's Amazonas state attracted the attention of researchers in the beginning of the century and caused a lively discussion. Besides its significant syntactic peculiarities it also has striking semantic specificity in such areas as colour, kinship and quantity.

The last area is of particular interest. Pirahã has no cardinal or ordinal numbers, and Pirahã people do not know numeracy. A major scientific debate is associated with the interpretation of these facts. The key questions are: can we talk about the correlation of these facts (i.e., about the influence of language on thought), and whether it is possible to claim that Pirahã people do not have corresponding cognitive abilities.

Metamathematical Investigations on the Theory of Grossone

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Keywords. Logical theories; consistency; Grossone.

We will present Sergeyev's Grossone Theory as described in [1] or [2] as a formal system, stating its axioms for the natural numbers in the predicative second order language. We will discuss the possibility of interpreting his additional postulates as metamathematical constraint.

The formal theory is shown to be consistent by an application of the logical compactness theorem, without any reference to non standard analysis. It is also a conservative extension with respect to arithmetic, but this is not relevant, since the interesting results involve the use of the new constant ①.

Since ① is meant in particular to measure the size of sets of natural numbers, the axiomatization of its theory cannot be restricted to a first order language. Predicative second order logic should however suffice, and its logical strength is not greater than first order, only the expressive power.

We will address open problems concerning definability (of sets) in this theory.

We will consider in subsequent work Grossone theory as a theory of real numbers, but will try already to indicate how the main results extend to the larger setting.

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Global Optimality Conditions in Non-Convex Optimization and Related Issues

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In this talk we are going to present recent results regarding global optimality conditions for general non-convex optimization problems. First we are going to discuss complexity issues regarding the existence of points satisfying optimality conditions and the connection to complementarity problems. In addition, we are going to discuss surprising connections between optimality conditions and continuous formulations of discrete optimization problems.

In the second part of the talk we are going to discuss our recent result regarding optimality conditions of locally Lipschitz functions. Namely, we show how the necessary conditions for a local minimum can be used to obtain a sufficient optimality condition of first order for a global minimum of a locally Lipschitz function on a closed convex set in a Banach space.

Emerging Utility

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Utility function seems to be the most disputable concept in the realm of mathematical economy. Analysis of prices and purchases on commodity markets add to this discussion the next paradoxical result: on one hand, behaviour of individual or household which has will and reflection CANNOT be described as maximization of any utility function, one the other hand, behaviour of large group of individuals (say, customers of one shop) which has no common will and reflection often CAN be described as maximization of some utility function.

To illustrate this thesis we consider simplified model of commodity market where we deliberately deprive consumers of information and options, which they usually have. Assume that there is the only trader in the market, which has stocks of different commodities. Customers come at random moments and ask to sell a certain bundle of commodities for certain amount of money. Stocks of trader are replenished with continuous steady flows. The trader knowing the distribution of orders and current stocks accepts or rejects the next order so as to maximize the expected discounted profit.

The optimal behaviour of the trader generates ergodic Markov process of changes in stocks. We investigate it by asymptotic expansion of the Bellman equation by small parameter ε which is the ratio of discounted factor to mean frequency of orders.

Consider what we will observe in our model market when replenish velocity $\mathbf{v}$ changes quasi-stationary. Stocks oscillate randomly in the vicinity of relative width $\varepsilon^{\frac{2}{3}}$ around equilibrium level $\bar{\mathbf{Q}}$ which connected with $\mathbf{v}$ by asymptotic relation $\bar{\mathbf{Q}} \sim (\mathbf{v}/\varepsilon)^{\frac{2}{3}}$. So the typical size of stocks is relatively large and depends on flow by the low often used in the inventory control theory. The trader selects proposals by cutoff price $\mathbf{p}(\mathbf{Q})$. In the typical vicinity of stocks the cutoff price depends on stocks unexpectedly week. $\mathbf{p}(\mathbf{Q}) = \bar{\mathbf{p}} + O(\varepsilon^{\frac{2}{3}})$. This means that the model explains usual economic preproposition on linear dependence of value on volume.

Collecting the trade statistics of average sales and equilibrium prices at different $\mathbf{v}$ we will see that this statistics may be rationalized by utility function $U(\mathbf{z}) = \min\limits_{\mathbf{p}} \left\{ \mathbf{p}\cdot\mathbf{z} + \int\limits_0^\infty d\mathbf{w} \int\limits_{\mathbf{p}\cdot\mathbf{w}}^\infty dW\, h(W,\mathbf{w})\, (W - \mathbf{p}\cdot\mathbf{w}) \right\}$, where $h(W,\mathbf{w})$ is the probability that the next customer will try to buy a bundle $\mathbf{w}$ for money W.

Grossone Infinity Computing: Foundations

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Keywords. Numerical infinities and infinitesimals; Infinity Computer; numbers and numerals; infinite sets.

This tutorial introduces a new methodology (different from non-standard analysis theories) allowing one to execute *numerical* (not symbolic) computations with finite, infinite, and infinitesimal numbers (see surveys [1, 2] and a semi-popular introduction in [3]). These numerical computations can be executed on a new type of a computational device – the Infinity Computer (see patents [4]). The new approach is based on the principle 'The part is less than the whole' introduced by Ancient Greeks and applied to all numbers (finite, infinite, and infinitesimal) and to all sets and processes (finite and infinite).

The new methodology examines in detail the difference between mathematical tools used to describe mathematical objects and the objects themselves. In particular, it is stressed that numerals we use to write down numbers (finite, infinite, and infinitesimal) are among our tools and, as a result, they strongly influence our capabilities in studying numbers. A variety of numeral systems including numerals used by Cantor and numerals introduced in [1–3] are compared from several points of view. The concept of *accuracy* of mathematical languages and its importance for a number of theoretical and practical issues regarding computations is discussed. Numerous examples and applications are given. The Infinity Calculator using the Infinity Computer technology is presented.

Acknowledgements. This study was partially supported by the Ministry of Education and Science of Russian Federation, project 14.B37.21.0878.

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Analysis on non-Archimedean Field Extensions of the Real Numbers and Applications

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Keywords. Non-Archimedean analysis; Levi-Civita fields; analytic functions; measure theory and integration; optimization; operator algebras; computational differentiation.

In this talk, we will give an overview of our work on non-Archimedean ordered field extensions of the real numbers that are real closed and complete in the order topology. The smallest such field, the Levi-Civita field $\mathcal{R}$ [1], is small enough to allow for the calculus on the field to be implemented on a computer and used in applications such as the fast and accurate computation of the derivatives of real functions up to very high orders [2].

We will summarize the convergence and analytical properties of power series, showing that they have the same smoothness behavior as real power series; and we will present a Lebesgue-like measure and integration theory on $\mathcal{R}$. Moreover, based on continuity and differentiability concepts that are stronger than the topological ones, solutions to one-dimensional and multi-dimensional optimization problems will be outlined.

A natural inner product can be defined on c_0, the space of null sequences of elements of $\mathcal{C} := \mathcal{R} + i\mathcal{R}$, which induces the sup-norm of c_0. Unlike classical Hilbert spaces, c_0 is not orthomodular with respect to this inner product, so we characterize those closed subspaces of c_0 with an orthonormal complement. We will present characterizations of normal projections, adjoint and self-adjoint operators, and compact operators on c_0 [3]. Then we will study in details the properties of positive operators on c_0.

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Constrained Global Optimization: Multiprocessor Approach

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Keywords. Global optimization; space-filling curves; parallel computations.

A collection of global optimization algorithms employing different types of a priory and accumulated information to boost the search for global optimum is presented in [1–4]. These schemes may easily be used as constituents for building some more sophisticated combined procedures that could be effectively accelerated being run on multiprocessor systems. Some of these possibilities are listed below.

If $\varphi(y)$ is a Lipschitzian function defined on the N-dimensional hypercube D then the N-dimensional global optimization problem by applying a Peano space-filling curve $y(x)$ can be reduced to a one-dimensional problem of minimizing $\varphi(y(x))$ over the interval [0, 1]. The reduced problem can be then solved by efficient algorithms [1, sec. 8.1]. Some of these algorithms allow effective parallelization [1, sec. 9.1–9.3]. Approximation techniques for computing $y(x)$ are also available [1, sec. 8.2]. To accelerate the search, a set of space-filling curves can be used [1, sec. 10.1] together with a smart parallel implementation [1, sec. 10.3].

Multi-dimensional global optimization problems with multiextremal partially defined constraints can also be reduced to a one-dimensional unconstrained problem [1, sec. 8.3] that can be then solved by the algorithm [4] allowing an effective parallelization, as well.

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Synchronization in Cellular Automata

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Keywords. Cellular automaton; firing squad synchronization problem.

Synchronization of large-scale networks is an important and fundamental computing primitive in parallel and distributed systems. We study a synchronization problem that gives a finite-state protocol for synchronizing cellular automata. The synchronization in cellular automata has been known as firing squad synchronization problem: FSSP, in which it was originally proposed by J. Myhill in the book edited by Moore [1964] to synchronize all/some parts of self-reproducing cellular automata. The problem has been studied extensively for more than fifty years [1, 2]. It is defined as follows: Given a one-dimensional array of n identical cellular automata, including a *general* at one end that is activated at time $t = 0$, we want to design the automata such that, *at some future time*, all the cells will *simultaneously* and, *for the first time*, enter a special *firing* state. The problem has been referred to as achieving a *macro-synchronization* in *micro-synchronization* system and *realizing a global synchronization using only local information exchange*. In this paper, we present a survey on recent advances in designing optimum- and non-optimum-time synchronization algorithms and their implementations for cellular arrays. Several simple, state-efficient mapping schemes are proposed for embedding 1D FSSP algorithms onto 2D, 3D and multi-dimensional arrays.

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Computations with Rational Numbers and Black Hole Formation Paradox

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Arbitrary real numbers are unobservable. Therefore the widely used modeling of physical phenomena by using differential equations, which was introduced by Newton, does not have an immediate physical meaning. Motivated by p-adic mathematical physics was suggested in [1, 2] that the physical meaning should be attributed not to individual trajectory in the phase space but only to probability distribution function. Even for the single particle the fundamental dynamical equation in the proposed "functional" stochastic approach is not the Newton equation but the Liouville equation or the Fokker–Planck–Kolmogorov equation. The Newton equation in functional mechanics appears as an approximate equation for the expected values of the position and momentum.

Applications of this non-Newtonian mechanics and to field theory and to the black hole formation paradox will be discussed. There is an astronomical evidence that many galaxies, including the Milky Way, contain supermassive black holes at their centers. However, a paradox occurs that for the formation of a black hole an infinite time is required as can be seen by an external observer, and that it is in contradiction with the finite time of existing of the Universe. We argue that to solve the paradox one can use the functional non-Newtonian mechanics. Probability of formation of a black hole for the external observer in finite time during collapse is estimated.

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Computing Sums of Conditionally Convergent and Divergent Series Using the Concept of Grossone

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Keywords. Summation methods; infinity; divergent series; conditionally convergent series; grossone.

Let $a_1, a_2, \ldots$ be a numerical sequence. In this talk we consider the classical problem of computing the sum $\sum_{n=1}^{\infty} a_n$ when the series is either conditionally convergent or divergent. We demonstrate that the concept of grossone, proposed by Ya. Sergeyev in [1], can be useful in both computing this sum and studying properties of summation methods.

First we prove that within the grossone universe, any rearrangement of a conditionally convergent series does not change the result of summation. This statement is then applied for computing sums of a large class of conditionally convergent series. We do that by splitting the original sum into the difference of two divergent sums with positive terms and expressing the result of summation of both divergent sums in terms of powers of grossone.

We then turn our attention to divergent series and demonstrate that the notion of grossone can simplify the exposition of some summation methods of divergent series as well as the analysis of these summation methods.

Some of the results discussed in this talk have been published in [2].

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Polymer Based Micro-Billiard Lasers: A Test-Bed in Nonlinear Physics and Applications

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Keywords. Open systems; micro-cavity; nonlinear dynamics.

The generic "billiard problem" is a paradigm of nonlinear mathematical physics, which connects to deep issues in quantum and wave physics all the way to quantum or wave chaos. It can be implemented in mechanics, optics or electromagnetism, either within classical or quantum mechanics, depending on experimental configurations and on the billiard length-scale. The elusive borders between wave and geometric optics on the one hand, and between quantum and classical mechanics on the other, exhibit deep analogies which can be both addressed in actual billiard-like physical systems. We will show the relevance in this context of micro-billiard shaped lasers [1–4] whereby spatially distributed modes can be connected to classical orbits within the semi-classical approximation, by use of Gutzwiller's celebrated "trace theorem", herein extended to open systems including chaotic ones. A number of interesting contours will be discussed, including stadiums, polygons (in particular squares and triangle) referenced to the Fabry-Pérot etalon cavity, where full fledged Maxwell-Helmholtz calculations on the one hand, closed orbital considerations on the other hand and last but not least experimental results are reconciled to provide consistent insights onto deep issues of current interest, some of which still elusive from mathematical and physical points of views, such as relating to diffraction from singularities.

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Regular Presentations

Unconditionally Stable Meshless Integration of Maxwell's Equations

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Keywords. Meshless methods; leapfrog ADI; Maxwell's equations.

Numerical solution of equations governing time domain simulations in computational electromagnetics, is usually based on grid methods in space and on explicit scheme for the evolution in time. A predefined grid in the problem domain and a stability step size restriction must be accepted severely limiting the applications. Evidence is given that efforts need for overcoming these heavy constraints. In solving Maxwell 's curl equations, by modeling interrelations between electric and magnetic fields, the authors developed a meshless method to avoid the need of information on the position among nodes scattered in the problem domain. Despite the good spatial properties, the numerical explicit integration used in the original formulation provides, also in a meshless context, spatial and time discretization strictly interleaved and mutually conditioned. In this paper a leapfrog formulation of the alternating direction implicit finite difference scheme for marching-on in time is combined with the meshless framework in space. The new formulation proposes a leapfrog form of the time advances equations, with implicit time field updating and by avoiding the computation of the mixed spatial derivatives. The new method not constrained by a gridding in space and unconditionally stable in time, is assessed by different numerical simulations.

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Convection in Semicircular Tubes

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Keywords. convection; semicircular; Nusselt number.

The purpose of this research is to study the problem of transient forced convection in a semicircular tube with constant wall temperature. The incompressible laminar flow is assumed hydrodynamically fully developed but thermally developing. An analytical exact solution of the velocity distribution of the flow field is used to numerically obtain the time developments of the thermal field. The results are presented in the form of velocity distribution, the time developments of isotherms, and Nusselt number development. The results are also verified and compared to relevant published literature.

Acknowledgements.

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Simulated Annealing for a Bi-Objective Trim Loss Problem with a Variable Large Object Length

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Keywords. Trim-loss or cutting stock problem; integer linear programming.

The trim-loss or cutting stock problem (CSP) is an important applied optimization problem. CSP assumes a given a number of standard sizes of long objects, and customer demands for different quantities of smaller pieces. A CSP solution specifies the number of smaller pieces cut from each large standard-size object. Of course, many smaller-piece cut combinations may not consume the full size of the larger objects, resulting in smaller, unused remainders called trim loss. The main objective of CSP is to minimize the total trim loss (wasted material) left over after cutting all larger objects necessary to satisfy customer orders. However, optimum solutions are difficult for practical, industrial-size CSP problems. As CSP is a complex, NP-complete optimization problem, heuristic techniques are usually used to solve large-size practical CSP.

One-dimensional problems (1D-CSP) involve cutting decisions on object lengths only, as in the case of paper and fabric rolls that have the same width. 1D-CSP models may consider either a single given size or a few given standards sizes for all available large objects. Previous 1D-CSP models assume these large-object sizes to be given constants. This paper presents a 1D-CSP model with a single but unknown large-object size, assuming this size to be a decision variable to be optimized. The primary objective is to minimize the total trim loss, and the secondary objective is to minimize the number of partially used large objects.

An integer linear programming (IP) model of the problem is formulated to determine the optimum number and size of the large objects, and the cutting pattern for each large object. As the optimum solution of this ILP model is difficult to obtain, a two-stage simulated annealing (SA) heuristic is developed to solve the problem efficiently. First, the First-Fit-Decreasing heuristic is used to generate initial solutions, and then SA is used to improve the solution. Numerical experiments are performed to demonstrate the effectiveness of this algorithm.

High Performance Computing Applied to a Multi-Objective Evolutionary Algorithm

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Keywords. Nonlinear multi-objective optimization; parallelism; facility location problems.

Many real-life problems include conflicting objectives. Recently, a new multi-objective evolutionary algorithm, called FEMOEA, which can be applied to many nonlinear multi-objective optimization problems, has been proposed. Its aim is to obtain a discrete approximation of the complete Pareto-front. FEMOEA has been compared to an interval branch-and-bound algorithm able to obtain an enclosure of the true Pareto-front as well as to the reference NSGA-II, SPEA2 and MOEA/D algorithms (see [1]). Comprehensive computational studies have shown that, among the studied algorithms, FEMOEA provides better approximations. The computational time needed by FEMOEA may be not negligible at all when the set approximating the Pareto-front must have many points, because a high precision is required. Furthermore, the computational resources needed may be so high that a PC may run out of memory. In those cases, parallelizing the algorithm and run it in a supercomputer may be the best way forward. In this work, a parallelization of FEMOEA, called FEMOEA-Paral, is presented. To show its applicability, a bi-objective competitive facility location and design problem is solved (see [2]).

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A Fuzzy Bayesian Classifier with Learned Mahalanobis Distance

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Keywords. Classifier; learning Mahalanobis distance; fuzzy c-means.

Recent developments and research show that a more general concept of a distance function in learning algorithms provides improved performance over classically used distance functions such as the Euclidean distance. One particular view is that one should consider side information such as specifying which pairs are similar and which are not. Xiang et al. (2008), for example, develop an algorithm to learn a Mahalanobis distance metric by supplying prior knowledge in terms of similar and dissimilar data pairs, which are called must-links and cannot links, respectively. The learned Mahalanobis distance then can be used in a clustering or classification algorithm. It is expected that the learned distance function will improve the performance of the algorithm.

In this paper, we consider a new classifier by applying the fuzzy c-means (FCM) clustering algorithm with a learned Mahalanobis distance. The algorithm for learning the Mahalanobis distance is almost the same as described in Xiang et al. (2008). One of the basic differences in our method is that the must-links and cannot-links are obtained directly from the data set as opposed to the approach in Xiang et al. (2008). This is achieved by using similarities between the data points. The classification is based on using fuzzy membership functions, which are constructed from the obtained clusters by using the learned Mahalanobis distance. The performance of the proposed classifier is analyzed by using some real data sets.

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Computational Modelling of the Biosensor with Competitive Substrates Conversion

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Keywords. Biosensor; modelling; competitive substrates conversion.

Biosensors are analytical devices used mainly for the recognition of the chemical substances in a solution to be analysed. Biosensors are widely applied in food, ecology, environmental and medicine industries [1]. Mathematical modelling is one of the most attractive solutions to understanding the peculiarities of the biosensors, which is a crucial step in their design and optimisation [2]

The purpose of this work was to develop mathematical as well as the corresponding numerical models of a mono-biosensor utilizing a competitive substrates conversion and to investigate the behaviour of the sensor at various sets of the models parameter values. The developed mathematical model is based on a system of reaction-diffusion equations with a non-linear reaction term:

$$v(t) = \frac{(V_1/K_1)S_1 + (V_2/K_2)S_2}{1 + S_1/K_1 + S_2/K_2},$$

where t is time, S_1 and S_2 are the substrate concentrations, V_1, V_2, K_1 and K_2 are the kinetic constants [3]. An enzyme layer, a dialysis membrane, a diffusion limiting region and a convective region are the regions describing the biosensors configuration. The corresponding computational model was developed by applying the Crank-Nicolson finite difference method [2].

The digital simulation showed complex behaviour of the biosensor at the different values of both concentrations of substrates and their corresponding maximal enzymatic reaction rates (V_1 and V_2).

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Parallel Global Optimization for the Problem of a Regional Economy Model Identification

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Keywords. Global optimization; nonconvex constraints; parallel computing; applied problems.

This study is related to the solution of the parameter identification problem for the mathematical model of a regional economy (on the example of the Nizhny Novgorod region). The approach to construction of a mathematical economy model developed in the Computing Centre of RAS [1] implies finding unknown parameters of the model by solving an optimization problem. This problem is multiextremal with a big number of parameters and constraints, complex black-box functions.

An efficient global optimization algorithm developed in the N. I. Lobachevsky State University of Nizhny Novgorod (UNN) combined with the scheme of separate consideration of constraints without penalty functions [2] was used for the solution of the mentioned problem. Herewith the solution of the multi-variable problem is reduced to the solution of an equivalent one-dimensional problem using Peano-type space-filling curves [2]. A parallelization scheme based on the evolvents set [3] was employed for organization of parallel computing. The problem was solved on the UNN cluster. Test computational experiments with the identified model proved the model efficiency.

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Discrete-Continuous Models and Optimization of Heterogeneous Systems

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Keywords. Heterogeneous System; discrete-continuous model; optimal control.

The practical needs of automation in various areas cause an increasing interest in models of heterogeneous systems. The study of such systems started in 1950 - 1970 from the works of E. Barbashin, S.V. Emelyanov, Y. Neumark, I. Flugge-Lotz, Ya.Z. Tsypkin, Yu.S. Popkov, V.I. Gurman, I.V. Rasina. Number of publications on this subject under the term "hybrid systems" as switching or impulse type differential systems associated with names of A.S. Bortakovskii, M. Branicky, S.N. Vassilyev, R.T.N. Cardoso, J. Lygeros, A.B. Kurzhanskii, and many others is steadily increasing. Many of them are connected with optimal control problems, when classic methods for homogeneous systems can not be applied directly.

Here an approach based on a hierarchical representation of heterogeneous systems and their decomposition into separate homogeneous subsystems is considered. Two-level model is constructed with continuous homogeneous processes at the lower level and discrete control of their switching at the upper level. Such model allows one to describe systematically the changing not only the structure, but also the order and even the nature of homogeneous subsystems. For this system the optimal control problem is stated and general and specific sufficient optimality conditions of Krotov type are obtained.

A series of approximate and numerical methods with a single iterative optimization procedure is proposed where only improvement operators in separate iterations differ. The proposed methods are based on the principle of local approximation by simplified constructions of global sufficient optimality conditions in the neighborhood of current iteration. This opens up many opportunities of constructing specific iterative processes in the unity of fundamental principles and program implementation.

In particular, an iterative method for linear discrete-continuous systems is constructed. This method is developed on the basis of sufficient conditions and Krotov minimax scheme of global improvement. Its effective application to the quantum systems control problems is demonstrated.

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Interpolation of Fuzzy Numbers

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Keywords. Interpolation formulas; fuzzy numbers; smoothing.

In this paper, we consider properties concerning approximation for fuzzy data by using cubic spline interpolation, monotone cubic interpolation and Lagrange interpolation. It is very useful for the scientific community in the area of smoothing approximation with fuzzy numbers to determine the accuracy of the approximation results from a fuzzy data set. The comparison analysis of interpolation techniques is made for approximation of the membership function given on the finite member of point. Numerical examples are given to compare the behavior of these methods.

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Approximate Solution of Inverse Parabolic Problem

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Keywords. Inverse parabolic equation; unknown coefficients; homotopy analysis method.

In this paper, an inverse parabolic equation is solved by using the homotopy analysis method (HAM) and the homotopy perturbation method (HPM). The approximation solution of this equation is calculated in the form of series whose components are computed easily. Homotopy perturbation method (HPM) is shown not always to generate a continuous family of solutions in terms of the homotopy parameter. By the convergence-control parameter this can however be prevented to occur in the homotopy analysis method (HAM). Illustrative examples are presented to exhibit a comparison between the homotopy analysis method (HAM) and the homotopy perturbation method (HPM).

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Test Rig Optimization and Block Loads

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Keywords. Discrete optimization; continuous optimization; multi-objective optimization; engineering; linear elasticity.

Durability is one of the most important physical properties of automobile component. The typical procedure to assess its structural damage is the test drive, which is expensive, takes a lot of time and can be done only after the whole automobile is assembled. One of the possible ways to make the tests cheaper and faster is to use the testing stands, where the so-called *actuators* will create load signals to emulate the real test drive damage.

The problem to find the optimal test rig configuration and actuators load signals can be formulated as an optimization problem, which includes multi-objective, discrete and continuous parts.

We introduce a new model of the problem, which avoids the necessity to deal with the rainflow-counting method – an algorithm, which converts irregular signal into the block signal. The model assumes block structure of the load signals from the beginning, which highly reduces the complexity of the problem without the feasible set decrease. Also we optimize with respect to the actuators position, which makes it possible to take moments of force into account and thus extend the feasible set.

As a result, the new model gives significantly better results, compared with the current approach in the test rig optimization.

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Image Restoration from Poisson Data by an Inexact Bregman Iteration Scheme

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Keywords. Inexact Bregman iteration; image restoration; Poisson noise.

The well-known Bregman iteration has been used in image restoration problems to obtain a contrast enhancement [1, 2]. Any iteration of this scheme requires to exactly compute the minimizer of a function. However, in some image reconstruction applications, it is either impossible or extremely expensive to obtain exact solutions of these subproblems. In order to improve the efficiency of the method we propose an inexact version of the iterative procedure where the *inexactness* in the inner subproblem solution is controlled by a criterion that preserves the convergence of the Bregman iteration and its features in image restoration problems. In particular, the method allows to obtain accurate reconstructions also when only an overestimation of the regularization parameter is known. The introduction of this inexactness allows to address image reconstruction problems for data corrupted by Poisson noise also when only an overestimation of the regularization parameter is known.The introduction of the *inexactness* in the iterative scheme allows to address image reconstruction problems from data corrupted by Poisson noise, exploiting the recent advances about specialized algorithms for the numerical minimization of the generalized Kullback–Leibler divergence combined with a regularization term. The results of several numerical experiments enable to evaluate the proposed scheme for image deblurring or denoising in presence of Poisson noise.

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FPGA-Based Calculator Using a CNN-UM Approach for Dynamical Systems Investigation

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Keywords. CNN; parallel computing; KdV; FPGA.

This describes a distributed computing system, called DCMARK, aimed at solving partial differential equations at the basis of many investigation fields such as Solid State Physics, Nuclear Physics and Plasma Physics. This distributed architecture is based on the Cellular Neural Network (CNN) paradigm which allows to divide the differential equation system solving into many parallel integration operations to be executed by a custom multiprocessor system. We pushed the number of processors to the limit of one processor for each equation. In order to test the present idea, we chose to implement DCMARK on a single FPGA, designing the single processor in order to minimize its hardware requirements and to obtain a large number of easily interconnected processors. This approach is particularly suited to study the properties of one-, two- and three-dimensional locally interconnected dynamical systems. In order to test the computing platform, we implemented a 200 cells, Korteweg de Vries (KdV) equation solver and performed a comparison between simulations conducted on high performance PC and on our system. Since our distributed architecture takes a constant computing time to solve the equation system, independently of the number of dynamical elements (cells) of the CNN array, it allows to reduce the elaboration time more than other similar systems in literature. To ensure a high level of reconfigurability, we designed a compact System on Programmable Chip (SoPC) managed by a softcore processor which controls the fast data/control communication between our system and a PC Host. An intuitively Graphical User Interface (GUI) allows to change the calculation parameters and plot the results.

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A Semi-Implicit Time-Splitting Scheme for Atmospheric Modeling

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Keywords. Atmospheric modeling; semi-implicit schemes; time-splitting methods.

The atmosphere is a complex system whose dynamics include the processes of different space and time scales. The most complete equations of the dynamical part of the atmospheric motions are the fully compressible nonhydrostatic equations based on the laws of conservation of the momentum, mass and energy for compressible inviscid ideal gas. As it is shown by the linear analysis, these equations support the three main types of atmospheric waves: acoustic, gravity and inertial waves. In addition to the distinct physical origin, these waves can also be differentiated according to the two features: the propagation speed and energy contribution. Acoustic waves propagate in the atmosphere with highest velocities, but their energy is negligible, the inertial processes are the slowest and the most valuable in energy spectrum, and the gravity waves occupy intermediate position both in propagation speed and energy contribution. Only the inertial processes are directly related to the main large scale atmospheric systems, which means that for the purpose of weather prediction the nonhydrostatic equations are a stiff system.

In this study, a semi-implicit time-splitting scheme is proposed for the nonhydrostatic atmospheric model. The fast acoustic and gravity waves are approximated implicitly, while slow advective terms and Rossby modes are treated explicitly. Such time approximation requires solution of three-dimensional elliptic equations at each time step. Efficient elliptic solver is based on decoupling in the vertical direction and then splitting in the horizontal directions. Stability analysis of the scheme shows that the time step is restricted only by the maximum velocity of advection and does not depend on speed propagation of the fast waves. The performed numerical experiments show computational efficiency of the designed scheme and accuracy of the predicted atmospheric fields.

On Stability of Semi-Implicit Schemes for Atmospheric Models

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Keywords. Atmospheric models; semi-implicit schemes; numerical stability.

The stiffness and nonlinearity of the mathematical models of atmospheric dynamics strongly affect the choice of the numerical methods used for computation of approximate solutions to the evolutionary equations. On the one hand, explicit schemes are rarely employed because of excessive restriction on the time step, which reflects the presence of the fast acoustic and gravity waves. On the other hand, the fully implicit schemes are not used due to complexity of nonlinear systems arising at each time step. Hence, the most popular approach for construction of numerical schemes is semi-implicit time differencing with implicit discretization of the linear terms responsible for fast waves and explicit treatment of the remaining part. Usually, only some linear terms with constant coefficients are approximated implicitly in order to ensure an efficient solution of the equations for implicit part, still using sufficiently large time steps.

There are many physically reasonable ways to choose the terms to be treated implicitly. However, some of these natural choices lead to the instability of numerical integration. The problem is related to the part of equations responsible for fast waves and it can result in unstable scheme for any choice of the time step. This behavior is caused by explicit approximation of the deviations from the reference vertical temperature profile. In this study, we derive the stability criterion in the terms of the vertical lapse rates of the reference and actual vertical profiles. In the case of specific vertical grids, we show that the obtained criterion is necessary and sufficient for the stability of numerical integration.

Limited-Memory Methods with Shape Changing Trust Region

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Keywords. Large-scale unconstrained optimization; limited-memory; quasi-Newton methods; trust region.

Limited-memory quasi-Newton methods and trust-region methods represent two efficient approaches used for solving unconstrained optimization problems. A straightforward combination of them deteriorates the efficiency of the former approach, especially when the problems are of large scale. For this reason, the limited memory methods are usually combined with a line-search. The trust region is usually determined by a fixed norm, typically, scaled l_2 or l_∞ norms.

We present a trust-region approach where the model function is based on a limited-memory quasi-Newton approximation of the Hessian, and the trust region is defined by a special norm. Since this norm depends on certain properties of the Hessian approximation, the shape of the trust region changes with every iteration. This allows for efficiently solving the subproblem.

We prove global convergence of our limited-memory methods with shape changing trust region. We also present results of numerical experiments that demonstrate the efficiency of our approach in the case of large-scale test problems.

RUSICA: A Model for Sandy Shore Evolution

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Keywords. Modelling and simulation; cellular automata; coastal erosion.

Sand erosion is spreading due to climatic change and contrast actions can be planned by computer simulations. RUSICA [1] is a developing model for such a complex phenomenon. It is based on Macroscopic Cellular Automata (MCA) [2] methodology, for investigating natural macroscopic systems, that evolve mainly on the base of local interactions of their constituent parts. MCA are an alternative approach to PDE for developing model in incremental way in order to operate on different specification levels to be compared to experimental data. That permits to capture important elements for intervention in particular cases, as at Porto Cesareo coast in the Italian Apulia Region, 2011, where an efficacious action adopted some MCA suggestions. $RUSICA =< R, X, S, P, \gamma >$ in this successive version [1] is a three dimensions MCA, where R defines the space portion, tessellated in regular hexagonal cells, where dynamical system evolves. X is the cell neighbouring conditions, specified by its adjacent cells. S is the set of cell states, that describe the features of the corresponding portion of space in terms of substates, the third dimension is implicit in some substates. Relevant cell substates are altitude, water depth, sand layer thickness, average kinetic energy of sea water, sea water average sand concentration, suspended sand flows. P is the set of global parameters, they include the temporal MCA clock, the cell apothem, the energy reflection and transmission coefficients, parameters of sand mobilization and deposit. The transition function γ computes sand erosion, transport and deposition. Interesting simulation results for ideal and simplified real cases encourage us for a further model improving.

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Average-Case Analysis of Optimization of Brownian Bridge with Normal Measurement Error

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Keywords. Optimization; average-case complexity.

We consider the problem of approximating the minimum of a continuous function using only sequentially chosen function evaluations corrupted by independent normally distributed noise. For this problem an average-case complexity analysis is interesting. We take as probability model for the unknown function the Brownian bridge. We describe an optimization algorithm, and establish that the error converges to zero at the optimal rate up to logarithmic factors.

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Product Rules Over The Square of Weakly Singular Double Integrals

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Keywords. Double integrals; numerical integration; product rules.

Double integrals of the form

$$\int_0^1 \int_0^1 \log|x-y| f(x,y)dxdy, \quad \text{or} \quad \int_0^1 \int_0^1 \frac{\log|x-y|}{\sqrt{xy(1-x)(1-y)}} f(x,y)dxdy,$$

are of interest in the linear theory of the aerodynamics of slender bodies of revolution [1].

In this talk we consider the double integrals of the form

$$\int_{-1}^1 \int_{-1}^1 k(|x-y|) f(x,y)dxdy, \qquad |x|,|y| < 1,$$

with $k(|x-y|) = |x-y|^\nu$,or $k(|x-y|) = \log|x-y|$and the function $f(x,y)$ is a smooth function on $[-1,1]^2$. In this paper we consider product rules of interpolatory type, based on suitable Jacobi zeros.

A different approach was recently proposed in [2], but the numerical method presented in the paper requires more computational efforts.

For the proposed method convergence results are proved and numerical tests are given.

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Dynamical Systems and Low Discrepancy Sequences

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Keywords. Uniform distribution; Kakutani-Fibonacci sequence; ergodic theory; interval exchange; discrepancy.

In this talk we show how to construct a family of uniformly distributed sequences of points in dimension one by means of suitable iterates of an ergodic interval exchange constructed ad hoc. The construction resembles the one used by von Neumann and Kakutani when they obtained the well known van der Corput sequence of points as the orbit at the origin of an ergodic transformation, known as the *von Neumann-Kakutani odometer* [3]. This recent result is the starting point of several investigations in higher dimensions (and the possible application in Quasi-Monte Carlo methods), among which we mention the first positive attempt of giving sufficient conditions for the uniform distribution of the *multidimensional LS-sequences of points* in the hypercube [4].

More precisely, we start from the Kakutani α-sequence corresponding to the inverse of golden ratio and we call it the *Kakutani-Fibonacci sequence of partitions*. This sequence belongs to a countable family of low discrepancy sequences of partitions introduced in [1]. To this sequence of partitions we associate an ergodic interval exchange (which we call the *Kakutani-Fibonacci transformation*) using the so called "cutting-stacking" technique.

We prove that the orbit of the origin under this map coincides with a low discrepancy sequence (which we call *Kakutani-Fibonacci sequence of points*), which is one of the possible reordering of the left-end points of the intervals of the *Kakutani-Fibonacci sequence of partitions*. The *Kakutani-Fibonacci transformation* is actually uniquely ergodic [4], hence the orbits of all the points in the unit interval are uniformly distributed.

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Analysis of Multi Step Exponential Signal Based on Prony-Like Method and Sliding Window

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Keywords. Multi step exponential signal; delay estimation; Prony-like method.

In the generation of exponential signal for testing electronic devices [1], causes occur that introduce distortion from the theoretical one. In [1, 2], the numerical procedure based on Prony-like method is pointed out to evaluate the parameters of the multi exponential function modeling the distorted signal. The procedure is based on the assumption that no constant component is part of the signal.

In the case of multi step exponential signal, i.e., the superposition of constant component and exponential signals starting in delayed time instants, the Prony-like method fails. The solution proposed in the research concerns with the use of iterative procedure based on Prony-like method and sliding observation window on the acquire signal. The Prony-like method estimates the parameters of the multi-exponential function inside the window and proper criterion is inferred to evaluate the delayed time instant of each exponential function.

In particular, if there are some component signals that have constant trend in the window, the estimated parameters are not coherent with their waited values and by sliding the observation window they are highly changeable. If all the component signals have exponential trend in the window, the estimated parameters are coherent with their waited value, and by sliding the observation window they are not highly changeable. By this analysis, the delayed time instant of each exponential function is estimated as the beginning of the window after that all the estimated parameters are not highly changeable.

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Stability and Hopf Bifurcation in a Delayed Ratio Dependent Holling–Tanner Type Model

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Keywords. Hopf bifurcation; stability; delay differential equations.

In this study, a delayed ratio dependent Holling–Tanner type predatorprey model is investigated. First, the local stability of a positive equilibrium is studied and then the existence of Hopf bifurcations is established. By using the normal form theory and center manifold theorem, the explicit algorithm determining the stability, direction of the bifurcating periodic solutions are derived. Finally, we perform the numerical simulations for justifying the theoretical results.

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A Classification of Cellular Automata Using Grossone

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Keywords. Cellular automata; Grossone; classification.

Cellular automata, originally introduced by von Neuman and Ulam in the 1940's, are discrete dynamical systems that are known for their strong modeling and self-organizational properties. Defined on an infinite lattice (in the one-dimensional case, the integers), even starting with complete disorder, the evolution of cellular automata, under repeated iterations, can generate organized structure. As with all dynamical systems, it is important to understand their evolutionary behavior. Hence it makes sense to develop a classification system based on their dynamical behavior.

The concept of classifying cellular automata was initialized, in the 1980's, by Stephen Wolfram. Through numerous computer simulations, Wolfram noticed that if an initial configuration (sequence of elements of a given finite alphabet) was chosen at random the probability is high that a cellular automata rule will fall within one of four classes. Robert Gilman later proposed a more rigorous probability measure/topological classification scheme for one-dimensional cellular automata. Gilman's classification was based on the probability of finding another sequence that stays arbitrary close to a given initial configuration.

This work provides an application of the Infinite Unit Axion and Grossone to the development of cellular automata to provide a new and rigorous classification scheme. In the traditional sense, the space of all infinite sequences of elements taken from a finite alphabet (the domain space of cellular automata) is uncountable. However, the Infinite Unit Axiom provides the computational power for counting the number of sequences that stay infinitesimally close to a given sequence, under iteration (evolution) of a cellular automaton rule. Hence one-dimensional cellular automata are partitioned into three classes, whereby each class corresponds to the number of sequences that stay infinitesimally close to an initial configuration.

An AMG Based on Compatible Weighted Matching for Image Segmentation

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Keywords. Algebraic multigrid; compatible relaxation; weighted matching; image segmentation.

Image segmentation addresses the problem to partition a given image into its constituent objects and then to identify the boundaries of the objects. This problem can be formulated in terms of a variational model aimed to find optimal approximations of a bounded function by piecewise-smooth functions, minimizing a given functional [1]. The corresponding Euler equations are a set of two coupled elliptic partial differential equations, one of which has discontinuous and varying coefficients. Numerical solution of the above system often relies on iterative methods, such as Gauss-Seidel or gradient descent coupled with semi-implicit or implicit discretization schemes, with low convergence rates. Faster and scalable solution are needed for large-scale applications, such as that arising in high-throughput screening platforms for computational biology. In this work we focus on the application of a new Algebraic Multigrid Method (AMG), recently proposed for linear systems arising from highly anisotropic elliptic partial differential equations, to the sequence of coupled systems arising in image segmentation by numerical solution of the Ambrosio-Tortorelli approximation of the Mumford and Shah model. The AMG applies a pairwise aggregation scheme based on weighted matching in a graph and on principles of compatible relaxation, which replace the commonly used characterization of strenght of connection among variables in both the coarse space selection and in the interpolation scheme [2]. We discuss convergence results and computational cost of the method in the analysis of 2D gray-scale images of embryonic stem cells colonies.

This work is a joint work with P. S. Vassilevski, Center for Applied Scientific Computing, LLNL, Livermore, CA, USA.

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Enhancing the Approximation Order of Local Shepard Operators by Hermite-Birkhoff Polynomials

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Keywords. Combined Shepard operators; Hermite-Birkhoff interpolation.

In connection with the problem of Scattered Data Interpolation, the procedure established in [1] is used in the case of local Shepard operators to retain the interpolation condition of Shepard-Taylor operators and to enhance, at the same time, its algebraic precision [2]. This procedure is based on the association of each sample point with a triangle with a vertex in it and other two vertices in its neighborhood, to reduce the error of special bivariate interpolating polynomials based on the vertices and used in combination with local Shepard operators. In [3, 4] the same procedure is applied in presence of lacunary data, i.e., when supplementary derivative data at each sample point are given, but not necessarily in successive order. In particular, the special cases of Lidstone interpolation and Complementary Lidstone interpolation have been considered and different operators for interpolation of scattered data have been obtained: the Shepard-Lidstone operator interpolates functional evaluations and all even order derivatives up to a fixed order at each sample point while the Shepard Complementary Lidstone operator uses and interpolates functional evaluations in some points and odd order derivative data in all points up to a fixed order. Here we approach the more general case of lacunary data of Hermite-Birkhoff type.

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The Majorizing Functions Approach in Inverse Problems

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Keywords. Inverse problems; computed tomography; optimization.

Most inverse problems could be modeled by the optimization of functions that are decomposed as a sum of two parts: one related to the consistency of the equations, that should be in principle satisfied, considering noise in data, and the other to prior information, not contained in those equations. In [1], we introduced a Majorizing Functions Approach (MFA), that simplifies the regularized optimization problem arising in Emission Computed Tomography (ECT), by separating its variables. This was later extended in a general context by K. Lange and other authors [2]. Recently, the explosion of articles on Compressed Sensing (CS) increased the importance of considering nondifferentiable priors. In this work we further extend the MFA, its relationship with projections in special measures of information, dealing also with the nondifferentiable case, improving on previous results and widening its range of application. Our reference inverse problem, illustrating the methodology, is ECT, as in [1].

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A Fast Algorithm for the Treatment of Integer Data in $\mathbb{Z}/p\mathbb{Z}$

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Keywords. Modular arithmetic; polynomial interpolation; numerical linear algebra.

The resolution of polynomial interpolation problems with integer coefficients directly involves the problem of the inversion of a Vandermonde matrix defined over the algebraic field $\mathbb{Z}/p\mathbb{Z}$, for p appropriate prime number.
The fact that Vandermonde problems are usually ill-conditioned and that standard numerically stable methods in general fail to accurately compute the entries of the solution vector motivated in the past the search for explicit formulas to solve Vandermonde systems by computing the inverse of the Vandermonde matrix [1-3]. A special instance of inversion of the Vandermonde matrix, which hasn't yet been investigated, regards the calculation of the inverse matrix with integer coefficients in $\mathbb{Z}/p\mathbb{Z}$ of a Vandermonde matrix defined from a vector of distinct elements of $\mathbb{Z}/p\mathbb{Z}$.
The purpose of this paper is to demonstrate the possibility to invert a Vandermonde matrix with integer mod p coefficients and exactly compute the integer inverse matrix in $\mathcal{M}at(\mathbb{Z}/p\mathbb{Z})$ through the new fast algorithm In$\mathcal{V}$anderMOD.
The explicit formula derived for the integer inversion of Vandermonde matrices, which is a generalization to modular arithmetic of [1], entirely develops inside the field of the integers mod p, with due consideration to the operation of integer division. The inversion procedure In$\mathcal{V}$anderMOD is valid for any prime number p and competitive in terms of computational effort, since its computational cost is less than $\mathcal{O}(n^3)$.

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Measurement and System Analysis of a Set of Academic and Psychological Characteristics for the First Year Students

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Keywords. System analysis; measurement; academic marks; individualization of curricula.

A complex of tools for a system analysis of the knowledge assessment and psychological characteristics for the first year university students has been worked out at the Biological Faculty of the N. I. Lobachevsky State University of Nizhni Novgorod, Russia. This complex includes measurement of 10 traditional characteristics that reflect: a subject knowledge, job motivation, level of mental development, creative abilities, etc. The introduced methodology has been applied in practice on a group of 120 students. Since all parameters have different scales, for each student each parameter was expressed in percentage of the maximum allowing so to sum up all the characteristics and to obtain the final total score. It has been shown that the obtained value is highly correlated with the actual results of the first examination period.

The correlation analysis of the collected data has shown that among the 10 measured parameters the generalization ability and the level of the subject knowledge in Biology are the main ones. It is interesting that merging these two characteristics in the only one gives a new parameter that has a high predictive validity, as well. As a result, it has been proved in practice that it is possible to significantly simplify the procedure of measurement and predicting success of students. This can be done by passing from measuring 10 traditionally used parameters to only two giving so the possibility to use the introduced approach for creating individual curricula for students at universities.

Existence Results for Fractional Differential Equations with Weakly Contractive Mappings

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Keywords. Fractional differential equation; fixed point theorem; weakly contraction mappings; partially ordered sets.

In this work, we establish some existence and uniqueness results for a class of boundary value problems for fractional differential equations via weakly contraction mappings in partially ordered sets.

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Communication Spanning Tree Problem in Wireless Sensor Networks

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Keywords. Wireless sensor network; transmission range; spanning tree; energy consumption; approximate algorithms.

This paper deals with the transmission energy consumption minimization problem in wireless sensor networks (WSN) which is known as Min-Power Symmetric Connectivity Problem (MPSCP) [1]. Let WSN be represented by the n-node weighted undirected graph G where the nonnegative weight c_{ij} of each edge (i, j) corresponds to the energy that every node i and j consumes for data transmission. A modern sensor can adjust its transmission range, and then the problem is to find a transmission range for each element to minimize the energy consumed to support a connected subgraph of G. Mathematically MPSCP is to find a spanning tree $T \subset G$ which minimizes the objective $W(T) = \sum\limits_{i \in V} \max\limits_{j\ (ij) \in T} c_{ij}$.

In [1] proposed FPTAS for constructing 5/3-approximate solution, polynomial 11/6-approximate algorithm, and exact branch and bounds method which uses a new formulation in form of integer linear programming problem.

In [1] MPSCP was considered when the nodes are placed in the Euclidean space and induce strongly connected graph with minimal total communication energy consumption. Authors proposed a polynomial algorithm for one special case and proved NP-hardness of the problem in the three-dimensional Euclidean space.

We found special cases of polynomial solvability, shown that the min-weight spanning tree with edge's weights in segment $[a, b]$, is $\left(2 - \frac{2a}{a+b+2b/(n-2)}\right)$-approximate solution, and the problem of constructing a 1,00048-approximate solution is NP-hard. Additionally, we proposed new polynomial heuristic algorithms and performed a representative simulation which demonstrates their high efficiency.

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Calculation of a Solution of Fourth-Order Initial Boundary Value Problem with Impulse

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Keywords. Fourth-order boundary value problem; transmission conditions; eigenvalues; eigenfunctions.

The following fourth-order partial differential equation

$$\rho(x)\frac{\partial^2 u(x,t)}{\partial t^2} + \frac{\partial^4 u(x,t)}{\partial x^4} = 0 \ \ (x \in (0,a) \cup (a,b), \ \ t > 0),$$

is considered in the paper. Here a, b are given positive numbers; $\rho(x) = \rho_1^4$ for $x \in [0,a)$ and $\rho(x) = \rho_2^4$ for $(a,b]$, where ρ_1, ρ_2 are given positive numbers. The main topic of the study is calculation of a solution of the considered equation subject to initial data, boundary and transmission conditions. The Fourier method is applied for solving this problem. The main step of this method is derived from eigenvalues and eigenfunctions of the fourth-order boundary value problem for some ordinary differential equation with piecewise constant coefficient. This paper continues the study from [1, 2].

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Applications of Grossone in Modern Theoretical Gravity

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Keywords. General relativity; mathematical physics; discretization.

We discuss a number of possible applications of Grossone methodology [1] to General Relativity (GR) together with its extensions [2–4]. As is well known one of the main problems of GR is quantization: the theory, as it is, is not renormalizable "tout-court", so that different quantization techniques should be used. It has been argued (first by Wheeler) that one should not only quantize the fields of gravity but also the Spacetime itself. Since then many attempts to quantization have flourished and most of them are based on suitable discretization procedures that often require to handle infinitely many pieces of Spacetime and/or infinitely many localizable notions. Among them we mention: 1) so-called "Regge Calculus", whereby techniques of static triangulation are required; 2) so-called "dynamic triangulation" that allows more flexible triangulations in which lengths are not rigidly fixed; 3) loop quantum gravity, whereby Spacetime is replaced by an appropriate "spin foam"; 4) path functional integration "à la Feynmann", where integration is performed along paths in Superspace. In these cases the use of infinities and of infinitesimals according to [1] (that allows one to perform calculations which resemble very much the techniques of traditional arithmetics but avoid a number of summation and probability difficulties) should be rather fruitful and could reasonably lead to a number of surprising simplifications in cumbersome calculations. The same techniques should find application in other fields of mathematical Physics that require handling denumerably infinite families of objects, such as: 1) Statistical Mechanics; 2) Quantum Mechanics; 3) Path Integral; 4) Renormalization Groups; 5) Lattice Field Theories.

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Observing Turing Machines Through the Lens of the Grossone Methodology

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Keywords. Observability of Turing machines; relativity of mathematical languages; infinite sequences; infinite sets.

The talk aims at investigating how the mathematical languages used to describe and to observe automatic computations influence the accuracy of the obtained results. In particular, we focus our attention on deterministic and non-deterministic Turing machines [1] and Multi-tape Turing machines which are described and observed through the lens of the recently proposed Grossone mathematical language [2]. It is strongly based on three methodological ideas borrowed from Physics and applied to Mathematics, namely: the distinction between the object (mathematical object in this context) of an observation and the instrument (mathematical language) used for this observation; interrelations holding between the object and the tool used for the observation; the accuracy of the observation determined by the tool.

Indeed, the Grossone language and the corresponding computational methodology, differently from the traditional one, makes it possible to measure the number of elements of different infinite sets [2] thus allowing to observe Turing machines with a higher accuracy with respect to that obtainable by using the traditional framework [1] giving so the possibility to better characterize and distinguish machines which are equivalent when observed within the classical framework. The talk studies deterministic and non-deterministic machines and enriches and extends the results presented in [3] by establishing a more accurate relationship between Multi-tape and Single-tape Turing machines.

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Effective Algorithms with Performance Ratios for Some Combinatorial Problems of Finding Several Discrete Structures in Complete Weighted Graph

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Keywords. Polynomial algorithms; performance guarantees; edge-disjoint Hamiltonian cycles; several minimum-weight cliques.

Typical combinatorial optimization problem, usually, associated with the search for the graph of a discrete structure. Examples of such structures are the Hamiltonian cycle, clique of a given size, spanning tree, matching, etc. Some of these problems are solved in polynomial time, but often such problems are NP-hard. Recently becomes urgent consideration problems in which you want to select in the graph a few (say, $m \geq 2$) such edge-or vertex-disjoint structures with extreme total weight. Most of these extensions are NP-hard problems. However, there are also polynomially solvable problems of this kind (for example, the problem of finding in complete undirected edge-weighted graph $m \geq 2$ edge-disjoint spanning trees of minimum total weight [1]).

This report focuses on problems of the rooting, clustering or covering type. As an example of these problems can result in a class of m-Peripatetic Salesman Problem, related to the search $m \geq 2$ edge-disjoint Hamiltonian cycles in complete edge-weighted grap with extreme total weight [2]. Here each route can be considered as a separate cluster of edges, and the set of routes is like covering the graph by $2m$-regular subgraphs of extreme summary weight. Another typical problem of this sort is the problem of finding in complete vertex- and edge-weighted graph several vertex-disjoint cliques of given size K with minimum total weight of the vertices and edges in the selected cliques. Here each clique can be considered as a separate cluster of edges and vertexes in the graph.

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Linearity Identification Tests for Cryptosystem Models

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Keywords. Discrete dynamical systems; identification tests; cryptographic transformers.

In this paper, we discuss the use of a linear mathematical model to describe cryptographic transformers that has a significant impact on the computation feasibility of a restoring inverter model and on the assessment of the resistance of a cryptographic system.

An algorithm for constructing a linear model of a cryptosystem encryptor is considered. Cryptographic transformers are described by discrete deterministic models such as autoregressive moving average models and digital Mealy machines. From the point of view of cryptanalysis, this kind of cryptosystem resistance testing may be classified as a cryptographic attack based on the plaintext and the corresponding ciphertext. The possibility of describing the cryptosystem decryptor using this linear model is tested.

Characteristic dependencies of the complexity parameter of the model of identified discrete dynamical systems on the length of text sequences are investigated.

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Computing Approaches for Solving Nonconvex Optimal Control Problems

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Keywords. Optimal control; computational technologies; applied problems.

Computing technologies developed by the authors [1, 2] allow one to solve problems of optimization in terms of nonlinear controlled systems of ordinary differential equations with parallelepiped constraints imposed on the control. By applying the mathematical reductions, it is possible to solve problems of a larger class: problems of parametric synthesis of optimal control, optimal control problems in systems with permanent delay and in singularly disturbed systems, problems bound up with approximation of reachable sets and integral funnels of controlled systems, problems of optimization for algebraic-differential systems and systems of semi-linear hyperbolic first-order equations.

To the end of solving auxiliary local optimal control problems, we have chosen a set of algorithms, which includes the methods based on Pontryagin's maximum principle, methods of conjugate gradients, quasi-Newtonian methods, Spectral Projected Gradient and Nesterov's ravine methods. The post-optimization analysis is conducted with the application of search algorithms. For the purpose of finding the global extremum, it is used a set of algorithms elaborated by the authors in recent years: the modifications of random multi-start method, methods based on approximation of the reachable set, methods of stochastic approximation [2], etc. The sphere of applications of developed computing approaches: problems related to flight dynamics, space navigation, mechanics, electroenergetics, robotics, medicine, ecology, biology, chemistry, nano-physics [3], etc.

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The Global Search in Lipschitzian Optimization Problems with Constraints Without Estimations of Lipschitz Constants

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Keywords. Global optimization; constraints; set of Lipschitz constants.

In article [1], the method DIRECT based on the special approach to a problem of global optimization of the Lipschitz objective functions without estimation of a Lipschitz constant has been proposed. Effective diagonal extension of the DIRECT is constructed in the monograph [2], and in the paper [3] a method of global search working with unbounded set of Lipschitz constants for gradients is proposed. New extensions of the DIRECT for a problem of Lipschitzian global optimization with constraints-inequalities are proposed in this report.

It is supposed that the Lipschitz constant L of the objective function belongs to an unbounded range, and the upper bound of a range of the Lipschitz constant values for constraints linearly depends on L. In the preliminary publication [4], new algorithms for a choice of evaluations are constructed and theoretically substantiated. These algorithms do not use any estimations of Lipschitz constants. New methods are partition ones. The one-point-based central partitioning scheme on hyperintervals is used. Hyperintervals for which there exist such values L that the least value of objective function minorant on this hyperinterval is smaller than in other hyperintervals, and inequalities for the least value of constraint function minorants are fulfilled, are undergone partitioning. Convergence of methods is proved, the results of computational experiments are given.

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Asynchronous Parallel Characteristical Algorithms for Global Optimization

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Keywords. Global optimization; characteristical algorithms; asynchronous parallel computations.

A wide class of parallel methods of global optimization based on asynchronous characteristical decision rule for search planning is considered. This class is a generalization of sequential prototype [1] and synchronous characteristical methods investigated in [2, 4]. Asynchronism is inherent to many computational approaches of complexity reduction in global optimization, for example, to nested optimization scheme [3, 4] or index method for solving constrained problems [4], and provides significant speedup in the course of optimization in comparison of synchronous algorithms.

General conditions of convergence for the asynchronous characteristical methods including sufficient conditions for finding out the globally optimal solution are theoretically substantiated. Theoretical results are illustrated with computational experiments concerned to optimization of multiextremal multidimensional test functions in the framework of nested optimization scheme in which asynchronous characteristical methods are used for solving nested subproblems. The results of experiments are in compliance with the theory and demonstrate the considerable advantage over synchronous characteristical algorithms.

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A Cellular Model for Tsunami Simulation

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Keywords. Cellular automata; modelling and simulation; tsunami.

Macroscopic Cellular Automata (MCA) [1] were developed for modeling and simulating natural phenomena evolving mainly on the base of local interactions. Such a methodology is alternative to the classic PDE approach and was applied especially to surface flows. In this work, we present the MCA model UNDATA [2] for tsunami simulation. UNDATA was developed in order to be coupled to SCIDDICA [3], an efficient MCA model for subaerial/subaqueous flow type landslides, when a displacement in water of significant volume occurs (but it works also for different generating causes).

UNDATA $= < R, X, S, P, \tau >$ is a three dimensional MCA, inspired largely to the TLM numerical method [4]. R defines the space portion, tessellated in regular hexagonal cells, where the dynamical system evolves. X is the neighbouring condition, specified for the generic cell by its adjacent cells. S is the set of cell states which describe the features of the corresponding portion of space in terms of substates. Relevant substates are "water depth", the "incident", "scattered" and "reflected" (six) pulses for the cell. P is the set of global parameters, they include the temporal MCA clock, the cell apothem, the reflection and the transmission coefficients. The transition function τ computes pulses from the sinking and movement of matter in water and their propagation, accounting for land inundation.

SCIDDICA-UNDATA was applied to the 1997 subaerial/subaqueous debris flow in Albano lake, Italy. First simulations show encouraging results regarding the general behavior of the model, even if highlighting the necessity to expand τ in future developments of UNDATA for a better approximation in simulations.

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Abstract Schemes of Iterative Optimization

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Keywords. Optimization; iterative improvement; extension principle; localization principle.

The lecture is devoted to abstract schemes of iterative improvement and optimization on the base of extension, localization and maximin principles, and to their general properties. Its main goal is to help with development of new concrete methods and algorithms for new problems with the use of visual examples.

The abstract optimization problem is stated as to find a minimizing sequence of a given functional in admissible set. Relative to above optimization problem is improvement problem which is solved to construct an improvement operator $\mathcal{F}(m)$ of any admissible element m and to use it in the iterative procedure

$$m^{(k+1)} = \mathcal{F}\left(m^{(k)}\right).$$

The extension principle is to replace the original constrained problem by a similar one but released of some constraints and modify the functional so that the new problem solution coincides with the solution of the original problem.

The localization principle [1] is to reduce the improvement problem to a simplified optimization problem as approximation of original one in the vicinity of improvable element m^{I}. It is achieved by direct contraction of the admissible set $\mathbf{D}$ or by penalization of large deviations from m^{I}.

Also special max-min principle [2] is used for nonlocal improvement.

To illustrate the constructiveness of above principles some new first- and second-order methods for the finite dimensional optimization problem and optimal control problem are developed.

General properties of thus constructed iterative procedures are considered. It is introduced the notion of *generalized non improvable element* and shown that any bounded improving sequence converges to such element.

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Multi-Experts Multi-Criteria Decision Making

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Keywords. Group decision making; argumentation networks; soft constraints.

Expert analysis and decisions are highly valued assets in a wide variety of fields, from social services to grant funding committees. However, the use of experts can be prohibitive due to either lack of availability or cost. As such, it is desirable to be able to replicate such decisions. However, there are many obstacles that impede an accurate simulation of expert decisions. For example, despite looking at the same information, two experts may disagree on the decisions. In addition, a single expert may make inconsistent decisions across similar scenarios.

In this work, we focus on multi-criteria decision making and in particular, in the case of multiple experts (ME-MCDM). We examine how multi-criteria decision making techniques can address the multi-experts dimension of the problem, as well as how argumentation networks can inform us about how to aggregate the multiple experts' decisions. Questions that we consider include: (1) How do we predict best decisions based on multi-experts' prior decision data? (2) How do we use the knowledge from (1) to be able to predict and diffuse disagreements in group decision making? We look at experts' decision data in the area of software quality assessment, and we analyze automated decisions that results from using non-discriminatory techniques (techniques that take all decisions – even conflicting – into account with the same importance). We reconsider these data, explore the use of argumentation networks, and reflect on the relevance of such approach. We report the results of our preliminary observations and we propose directions for future work.

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Infinity Computations in Percolation Theory Applications

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Keywords. Infinite sets; percolation; infinite cluster.

In the presentation, we consider a number of applications related to the theory of percolation. Site percolation, gradient percolation and directed percolation have been studied by applying the new computational tools [1–3]. It has been established that in infinite system phase transition point is not really a point as with respect of traditional approach. In light of new arithmetic it appears as a critical interval, rather than a critical point. Depending on "microscope" we use this interval could be regarded as finite, infinite and infinitesimal short interval. Using new approach we observed that in vicinity of percolation threshold we have many different infinite clusters instead of one infinite cluster that appears in traditional consideration. Moreover, we have now a tool to distinguish those infinite clusters. In particular, we can distinguish spanning infinite clusters from embedded infinite clusters. Than we consider gradient percolation phenomenon on infinite square lattice with infinitesimal gradient of critical parameter that changes linearly, accepting infinitesimal value in the first line of lattice cells and value equal to unit in the last, grossone line of lattice cells. We observe that diffusion front width in this case stretches for an infinite number of lattice spacing. And again this value could be regarded as finite, infinite and infinitesimal short depending on "microscope" we use.

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Self-Organized Bursting Dynamics of Neuronal Networks and Infinity Computations

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Keywords. Neuronal networks; bursting dynamics; cellular automaton networks.

In the presentation, we give several examples of the usage of the new numerical approach working with grossone in relation with the bursting dynamics of neuronal networks. Living neuronal networks in dissociated neuronal cultures are known to demonstrate highly robust activity patterns recorded in different experimental conditions. Such patterns are often treated as neuronal avalanches satisfying power scaling law and demonstrate a bright example of self-organized criticality in living systems. We consider a cellular automaton model related to the bursting dynamics using the new computational methodology. The introduction in these models new, computationally manageable notions of the infinity and infinitesimals gives a possibility to pass from the traditional qualitative analysis of the situations related to these values to the quantitative one. In the frame of the developed cellular automaton model we show that the interburst interval could be regarded as finite, infinite and infinitesimal short interval depending on resolution we use. Moreover, bulk number of spiking neurons involved in an arbitrary burst could be regarded as finite and infinitesimal values. The point of view presented in this paper uses strongly two methodological ideas borrowed from Physics: relativity and interrelations holding between the object of an observation and the tool used for this observation [1, 2].

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Vector Continued Fractions: Old Ideas, New Applications

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Keywords. Vector continued fractions; QD algorithm; difference operators; inverse spectral problem.

Vector continued fractions was introduced by Jacobi in connection with representation of algebraic numbers of higher degree by periodic code. The associated algorithm is called Jacobi-Perron algorithm and it is known to have many beautiful ergodic properties. From the other side it is known that Jacobi-Perron type algorithm cab be applied to the vector of power series and it produces a vector of simultaneous rational approximations with common denominator. This leads to the system of polynomials of simultaneous orthogonality (vector orthogonal polynomials) which are closely related with the spectral analysis of non symmetric difference operators (band Hessenberg operators). Jacobi-Perron algorithm in this case can be used to solve the inverse spectral problem [1]. In the present paper we discuss a new vector version of the well known QD algorithms. One version of vector QD algorithm was introduced in [2]. We use a different approach and show how it is connected with the inverse spectral problem for the class of operators studied in [3].

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Nonstandard Analysis on Surreal Numbers

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Keywords. Surreal numbers; nonstandard analysis.

Convay's [2] surreal numbers form a non-archimedean extension of the real line, defined by means of consecutive filling in all gaps. The "filling in" procedure goes on transfinitely so that all ordinal numbers are involved, and hence the result is a proper class rather than a set. It is known [1] that some elements of real analysis can be developed on the base of surreal numbers, albeit to much lesser extent than on the base of non-archimedean fields defined by methods of nonstandard analysis. Recent developments in the field of nonstandard analysis [4], as well as some modern results related to surreals themselves [3] allow to wiev surreals as a set-size saturated nonstandard extension of the reals. The talk will present recent results in this direction.

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Triangular and Square Triangular Numbers

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Keywords. Triangular numbers; square triangular numbers; perfect squares.

A number of the form $\frac{n(n+1)}{2}$ where $n \in Z^+$ is called a triangular number and the n^{th} triangular number is denoted by T_n. Triangular numbers which are also square numbers are called square triangular numbers and the n^{th} denoted by S_n. Square triangular numbers can be written as $S_n = s_n^2 = \frac{t_n(t_n+1)}{2}$ where s_n and t_n denote the sides of the corresponding square and triangle.

In this work, we deduced some new algebraic relationships on triangular, square triangular numbers, squares and triangles. Further, we established an important link between triangular and square triangular numbers.

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Solving Multi-index Linear Programs by Reducing to Tree-Like Networks

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Keywords. Linear programming; multi-index problems; transport type problems; reducing; flow algorithms.

Multi-index linear programs of the transportation type are considered. There exist many applied problems that can be formalized as multi-index problems [1]. One of approaches for solving such multi-index problems is based on reducing them to network flow problem. Used concept of reducibility is named $t_1 \mid t_2{-}equal \mid t_3{-}edge$ reducibility and described in [2].

In this paper as a network flow problem we consider min-cost flow problem in tree-like network, which will be denoted by W_{Tree}. Using the notation presented in [2] we denote the class of multi-index linear programs by $W(M)$, where $M \subseteq 2^{\{1,\dots,s\}}$ is the set which explicitly determines constraints of the problem, s is the number of indices.

Definition. A set $M \subseteq 2^{\{1,\dots,s\}}$, is said to be k-nested if there exists a partition of the set M into k subsets $M_i = \{f_1^{(i)}, \dots, f_{m_i}^{(i)}\},\ i = \overline{1,k}$, such that $f_j^{(i)} \subset f_{j+1}^{(i)}, j = \overline{1, m_i - 1}, i = \overline{1,k}$.

We prove the following necessary and sufficient condition of reducibility:

Theorem. For the class $W(M)$ to be $L \mid L - equal \mid L - edge$ reducible to the class W_{Tree}, it is sufficient that M is 1-nested.

Theorem. For the class $W(M)$ to be $t_1 \mid t_2 - equal \mid t_3 - edge$ reducible to the class W_{Tree}, it is necessary that M is 1-nested.

Reducibility results allow us to propose an algorithm for solving $W(M)$, where M is 1 nested. The algorithm consists of three main steps: reducing multi-index problem to min-cost flow problem in tree-like network, solving the flow problem and constructing the solution of original multi-index problem using the solution of flow problem. Proposed algorithm requires $O(n^2)$ computational operations, where n is the number of variables of the multi-index problem.

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A Computational Study of Option Replication Based on Riesz Space Theory

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Keywords. Strongly resolving markets; option replication; vector lattices.

In this talk we are going to present a new computational tool for option replication. In particular, a procedure is provided for computing the replicated exercise prices of a given portfolio. We highlight a matrix-based framework for analyzing option replication. The new matrix formulation allows the development of efficient computational methods in order to determine the replicated exercise prices of a given portfolio by using the theory of vector lattices and positive bases. Also, the notion of strongly resolving markets with respect to the positive basis of a minimal lattice-subspace Y of $\mathbb{R}^m$ is defined. It is proved that if the number of securities is less than half the dimension of Y, then not a single (non-trivial) option can be replicated. This result extends already known results regarding the notion of a market being strongly resolving. Both theoretical and computational methods are provided in order to establish criteria for the characterization of markets that do not replicate any option.

Our main objective is to make option replication computationally tractable and hence more viable as a financial tool.

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On Shifting of Methodological Metaphors or "Is Pure Sociology Possible?"

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Keywords. Philosophy of computer science; methodology; artificial intelligence; collective intelligence.

There are many issues related to the assessment of the ontological status of the program itself. The dual nature of computer program became linked with their simultaneous existence in the form of computer data. Data is a matter of abstraction, a kind of ideal object of computer science, getting its value during the process of formulation of the problem. This is why computer technology is so meaningful in the various scientific spheres.

If we take into account the cumulative nature of the development of computing technologies which makes material representation and abstractions storage possible, then we may clear the change of the so-called methodological metaphors (current regulations). Many scientific researches was triggered by the metaphor of "artificial intelligence". The notable philosophical challenge to the artificial intelligence was the attempt to solve so-called "understanding problem" (A. Turing, J. Searle). Machine learning itself was appeared as researching of algorithms to make transitions from one value to another in an optimal way.

Now this metaphor is shifted to the next one – the "collective intelligence", which defines the model of human interaction, mediated by computer communicative systems. The complexity of such researches is to evaluate the compatibility of the technical feasibility of mathematical models with the mental capabilities of the people themselves. However, the increased possibility of increasing the speed of communication does not provide the possibility of synthesizing something new. But the possibility of synthesis increases potentially, but not actually.

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Multistage Mathematical Programming Problems

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Keywords. Multistage mathematical programming problems; numerical integration of ordinary differential equations.

In this paper we consider the following problems:

$$Q_m(x_1, ..., x_m) = \sum_{i=1}^{m} c_i x_i \Rightarrow min, \tag{1}$$

$$X(m) = (x_1, ..., x_m) \in D_m = \{X(m) \in P_m \subseteq R^m | f_i(x_{i-1}, x_i) \leq 0, i = 1, ..., m\},$$

where the value of m is not supposed to be defined, but can be determined by problem solving. Here x_0 is interpreted as initial state of some system, x_m is an unknown final state, the condition $f_i(x_{i-1}, x_i) \leq 0$ gives the set G_i of possible system states at $i-$th stage (step) under the determined value of $x_{i-1} \in G_{i-1}$, where $G_0 = \{x_0\}$, i.e., it defines a point-to-set map at $i-$th stage, $\psi_i(x_i) = c_i x_i$ is a local criterion determined on G_i, $Q_m(x_1, ..., x_m) = \sum_{i=1}^{m} \psi_i(x_i)$ is an integral criterion determined on set D_m, $i = 1, ..., m$.

We will call these problems multistage problems. The multistage problem will be called M-problem if it satisfies the next condition: if the behavior of the system generated by the problem is optimal from the point of view of local criterion at each step then it is optimal from the point of view of integral criterion.

We have found sufficient conditions which guarantee that the problems (1) are M-problems. Moreover, both convex and non-convex cases have been considered. It has been shown that the problem of construction of approximately optimal procedure for numerical integration of ordinary differential equations are reduced to M-problems. Effectiveness of numerical integration formulas constructed in such a way is demonstrated by a model example.

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Hierarchical Tree Structure Systems with Costs

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Keywords. Hierarchical system; rooted oriented tree.

Let $G = (V, A)$ be the root oriented tree, $A \subseteq V^2$, $1, V_k, V_u$ – partitioning of set V: 1 is the tree root number, V_u is set of leaves numbers, V_k is set of numbers of intermediate; $A^{'}$ is a subset of A. Each node i is assigned pair B_i, C_i, $0 \le B_i \le C_i < \infty$, $i \in V$; each arc is assigned pair D_{ij}, E_{ij}, $0 \le D_{ij} \le E_{ij} < \infty$, $(i, j) \in A$. The problem is to find vector $\overrightarrow{x}$, $\overrightarrow{x} \in R^{|V|}$ and matrix $Y = \|y_{ij}\|_{(i,j)\in A}$, for which the following constraints are satisfied: $B_i \le \sum\limits_{j|(i,j)\in A} x_j \le C_i$, $i \in V_k \cup \{1\}$; $B_i \le x_i \le C_i$, $i \in V$; $D_{ij} \le y_{ij} \le E_{ij}$, $(i, j) \in A$; $\sum\limits_{j|(i,j)\in A} y_{ij} - f_i(\sum\limits_{j|(i,j)\in A'} y_{ij}) - x_i = 0$, $i \in V \setminus V_u$; and the criterion $F(\overrightarrow{x}, Y) = \sum\limits_{i\in V\setminus V_u} h_i f_i(\sum\limits_{j|(i,j)\in A'} y_{ij})$ takes its minimum value. Here h_i are rational numbers, $f_i(\sum\limits_{j|(i,j)\in A'} y_{ij})$ are some functions, which are determined for elements of set $L = \{i|(i, j) \in A^{'}, j \in V\}$, $i \in V \setminus V_u$.

Efficient solution algorithms of the posed problem have been developed in the case, when the functions $f_i(\sum\limits_{j|(i,j)\in A'} y_{ij}), i \in L$ are linear or quadratic. These algorithms are based on the method of border reduction [1].

Distribution similar resource in multilevel hierarchical tree structure with costs is occurred in following problems [1–3]: transporting of natural gas in multistrand gas main, distribution of financial resources, planning of off-take for production systems with multimode equipment.

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Optimal Control of Measure Dynamics

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Keywords. Optimal control; measure; dynamic systems.

Systems of probability and positive measures dynamics are widely used for the description of various nature processes. Physical laws are often formulated concerning density of distribution (weight, charge, etc). To consider the dynamics of the distributed and concentrated objects, equations for measures are required. The problem of optimum control for such processes is of great importance.

In this work, results on optimal control for probability and positive measures dynamics are presented. The general form of the equation of a probability measure dynamics is obtained. Theorems of resolvability of such equations are proved. The question of limit characteristics of the solution is considered. Necessary and sufficient conditions for the optimality of the probability measure dynamics are deduced. Various applications of the theory to specific problems in mathematical physics are considered.

The constructed theory allows to build new effective algorithms for the numerical solution of optimization problems. In this work, the problem of optimum control of heating process with phase restrictions is considered. For this classical problem a new solution in the form of feedback control is proposed. The efficiency of the proposed solution is confirmed by a numerical experiment.

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Usage of the Lipschitz Condition in Diagonal Global Optimization

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Keywords. Global optimization; Lipschitz condition; numerical methods.

Many practical decision-making problems can be stated as black-box global optimization problems. Their objective function is often Lipschitz (differentiable or not), multiextremal and hard to evaluate [1, 2]. Different approaches for solving these problems are discussed. They can be distinguished, e.g., from the following three viewpoints: (i) the way of obtaining the information about the Lipschitz constant; (ii) the rule used to select subregions for further partitioning; (iii) the strategy for partitioning the chosen subregions.

Several algorithms are analyzed and different constructive solutions to implement (i) – (iii) are discussed. Methods working with functions having the Lipschitz first derivative are also taken into consideration. The main attention is dedicated to diagonal algorithms, since they have a number of attractive theoretical properties and have proved to be efficient in solving applied problems. A number of diagonal multidimensional global optimization algorithms are reported. Results of numerical experiments on the GKLS-generator of classes of test functions with known local minima are presented and discussed [3, 4].

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Numerical Simulation of Bacterial Self-Organization in a Circular Container

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Keywords. Reaction-diffusion; pattern formation; simulation.

Various microorganisms and bacteria move toward food sources and away from dangerous substances [1]. Such directed movement plays a crucial role in a various biological processes and is called chemotaxis [2].

Recently, pattern formation of a luminous *Escherichia coli* colony in a circular container was modeled by reaction-diffusion-chemotaxis equations and various model modifications were studied to determine the suitable minimal model [3]. In this work, we investigate an extension of the proposed minimal model by incorporating a nonlinear gradient into dimensionless equations,

$$\frac{\partial u}{\partial t} = D\Delta u - \chi\nabla\left(\frac{u}{s}\tanh\left(\frac{s\nabla c}{1+s}\right)\right) + \gamma\alpha u\left(1-u\right),$$
$$\frac{\partial c}{\partial t} = \Delta c + \gamma\left(\frac{u}{1+\beta u} - c\right), \quad x \in \Omega, \quad t > 0,$$

where Ω stands for the circular domain, $u(x,t)$ is the cell density, $c(x,t)$ is the chemoattractant concentration, and γ describes the spatial and temporal scale.

By varying the input parameters the output results were numerically analyzed with a special emphasis on the influence of the nonlinear gradient on the spatiotemporal pattern formation. The mathematical model and the numerical solution were validated by experimental data [4].

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Global Optimization Methods for Lipschitz Functions Using Space-Filling Curves

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Keywords. Global optimization; space-filling curves approximations; set of Lipschitz constants.

Let us consider the following global optimization problem:

$$\min\{F(y) : \ y \in [a, b]\}, \tag{1}$$

where $[a, b]$ is a hypercube in R^N and $F(y)$ is a multiextremal function that satisfies the Lipschitz condition

$$|F(y') - F(y'')| \leq L\|y' - y''\|, \qquad y', y'' \in [a, b], \tag{2}$$

with a constant L, $0 < L < \infty$, generally unknown. In the literature, the problem (1), (2) is called *Lipschitz global optimization problem* and there exist a variety of numerical algorithms for solving this problem (see [1–4] and references given therein).

In this talk, we consider a powerful approach (see [4]) that uses numerical approximations of space-filling curves to reduce the original Lipschitz multi-dimensional problem to a univariate one satisfying the Hölder condition. In order to solve the problem (1), (2), we propose a new geometric method that uses, at each iteration, a number of possible Hölder constants from a set of values varying from zero to infinity.

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Three-Body Coulomb Systems: Bound *S*-States and Resonances

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Keywords. Three-body systems; binding energies; resonances.

A simple *Mathematica* [1] program for computing S-state energies and wave functions of three-particles systems subjected to the Coulomb interactions is presented. The relevant systems include two-electron atoms, molecular electronic ions and mesomolecular exotic species. In addition to the bound S-states the code enables one to compute the positions and widths of the lowest resonance, quasi-bound, states. The elegant technique derived from the classical papers of Pekeris [2, 3] represents a significant development of our previous work [4].

The basis functions are composed of Laguerre functions. The method is based on the *perimetric* coordinates and specific properties of the Laguerre polynomials. Direct solution of the generalized eigenvalues and eigenvectors problem is used, distinct from the Pekeris works. The complex rotation method is applied for calculating the resonance states.

The resultant wave functions have a simple analytical form, that enables calculation of expectation values of arbitrary physical operators without any difficulties. Only *one* mathematical parameter characterizing the basis size is required in the *input*. The other input parameters presenting masses and charges for the 3 particles are of the physical nature.

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An Algebraic Exposition of Umbral Calculus with Application to General Linear Interpolation Problem — A Survey

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Keywords. Sheffer polynomials; Appell polynomials; determinant.

Recently, various determinantal forms of sequences of Appell and Sheffer polynomials have been proposed. In particular, one of these allows an exposition of the main properties of classical umbral calculus, by using elementary tools of linear algebra. Even the computation becomes easier. Finally, an application to the general linear interpolation problem is made easy by the proposed determinantal form.

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Fractional Sensitivities of Semi-Simple Eigenvalues for Bifurcation Analysis

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Keywords. Sensitivity analysis; semi-simple eigenvalue; singular perturbations; stability domain; circulatory systems.

We perform high-order sensitivity analysis of eigenvalues and eigenvectors of linear systems depending on parameters. Attention is focused on double not-semi-simple and semi-simple eigenvalues, undergoing perturbations, either of regular or singular type. The use of integer (Taylor) or fractional (Puiseux) series expansions is discussed, and the analysis carried out both on the characteristic polynomial and on the eigenvalue problem. It is shown that semi-simple eigenvalues can admit fractional sensitivities when the perturbations are singular, conversely to the not-semi-simple case. However, such occurrence only manifests itself when a second-order perturbation analysis is carried out. As a main result, it is found that such over-degenerate case spontaneously emerges in bifurcation analysis, when one looks for the boundaries of the stability domain of circulatory mechanical systems possessing symmetries. A four degree of freedom system under a follower force is studied as an illustrative example.

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Strong Anticipation in Cellular Automata, Dynamical Systems and Neural Networks: Results and New Research Problems

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Keywords. Strong anticipation; cellular automata; multivaluedness.

The presentation is devoted to the description of rather new mathematical objects namely the system with anticipation. Mathematically such objects sometimes frequently have the form of advanced equations. Since the introduction of strong anticipation by D.Dubois the numerous investigations of concrete systems had been proposed. Some systems with anticipation had been considered earlier. But further development of the theory of anticipatory systems depends on the investigations of new examples of systems with anticipation and their new applications and interpretations. So in proposed paper the new examples of distributed and concentrated models with anticipation had been considered namely cellular automata, dynamical systems and neural networks etc. It is proposed the mathematical formulation of problems, possible analytical formulas for solutions and interpretations of presumable solutions. Complex behavior of such solutions is discussed. The main distinctive feature is presumable multi-valuedness of the solutions. Synchronization problems are discussed. Some consequences for computational science and their impact on natural sciences are proposed. Presumable role of 'grossone' in such models is discussed. A number of applications from physics, biology, and economy of proposed models are described. A list of further research problems is proposed.

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The Power of Grossone: From Bases to Hyperbolic Geometry

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Keywords. Grossone; bijection; hyperbolic geometry; tilings; tessellations.

In this talk, I shall look at the power of grossone to compute the number of elements in a set. In a first part, the question is considered in a very general setting. In particular, the role of bijections in the process of counting is analysed. In the second part, the counting is applied to an infinite family of tilings of the hyperbolic plane, after a detour to the Euclidean plane.

Most results of the talk can be seen in [1, 2].

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On the Constrained Mock–Chebyshev Least–Squares

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Keywords. Runge phenomenon; Chebyshev-Lobatto nodes; Mock–Chebyshev interpolation; simultaneous regression.

The algebraic polynomial interpolation on uniformly distributed nodes may be affected by the Runge phenomenon, also when the function to be interpolated is analytic. Among all techniques that have been proposed to defeat this phenomenon, there is the mock-Chebyshev interpolation which is an interpolation made on a subset of the given nodes whose elements mimic *as well as possible* the Chebyshev-Lobatto points [2]. In this work we will use the simultaneous approximation theory [1, 3] to combine the previous technique with a polynomial regression in order to increase the accuracy of the approximation of analytic functions. We will also give indications on how to select the degree of the simultaneous regression so as to obtain polynomial approximants good in the uniform norm [4].

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Constructive Lessons for Paraconsistency

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Keywords. Paraconsistent mathematics; constructive mathematics;

We discuss several cornerstone theorems of classical mathematics which come apart at the seams when viewed under the paraconsistent microscope. In particular, we investigate results concerning order and locatedness—a constructive concept—within a framework of analysis founded on a variety of paraconsistent logic. Practitioners of constructive mathematics have shown that there are crucial assumptions, implicitly made on the classical view (a result of the validity of omniscience principles), which separate out different versions of the same theorem. Here we shed light on what happens from the paraconsistent perspective. Again, we find (perhaps unsurprisingly) that one classical theorem has many paraconsistently distinguishable versions. But we find (perhaps surprisingly) that the constructive techniques that play a central role in highlighting these differences can often be adapted to paraconsistent modes of reasoning.

Computing Upper Bounds on the Constant of Interpolation

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Keywords. Computability; complex analysis; interpolation.

Let $\mathbb{D}$ denote the open disc whose center is the origin and whose radius is 1. Let $\mathbb{D}^\omega$ consist of all sequences $\{a_n\}_{n=0}^\infty$ such that $a_n \in \mathbb{D}$ for all n. Let $H^\infty(\mathbb{D})$ be the set of all bounded analytic functions from $\mathbb{D}$ into $\mathbb{C}$. For all $f \in H^\infty(\mathbb{D})$, let $\| f \|_\infty = \sup\{|f(z)| \ : \ z \in \mathbb{D}\}$. Let l^∞ denote the set of all bounded sequences of complex numbers. If $W = \{w_n\}_{n=0}^\infty$ is in l^∞, then we let $\| W \|_\infty = \sup\{|w_n| \ : \ n \in \mathbb{N}\}$. A sequence $Z = \{z_n\}_{n=0}^\infty$ in $\mathbb{D}^\omega$ is called *interpolating* if for every sequence of complex numbers $W = \{w_n\}_{n=0}^\infty$ in l^∞ there is a function $f \in H^\infty(\mathbb{D})$ such that $f(z_n) = w_n$ for all n. In this case, we say that f *interpolates* Z *to* W.

Suppose $Z = \{z_n\}_{n=0}^\infty$ is an interpolating sequence. It follows from the Open Mapping Theorem that there is a constant M such that for every $W \in l^\infty$, there is a function $f \in H^\infty(\mathbb{D})$ such that f interpolates Z to W and

$$\| f \|_\infty \leq M \| W \|_\infty .$$

The smallest such constant is called the *constant of interpolation* of Z and is denoted $M(Z)$.

Explicit bounds on $M(Z)$ are given in [1]. Inspired by these results, we consider the following questions.

1. Is there an algorithm that, given sufficiently good approximations to a sufficient number of terms of an interpolating sequence Z, produces an upper bound on $M(Z)$?
2. Is there an algorithm that, given a description of an interpolating sequence Z, produces an upper bound on $M(Z)$?

In the second question, we broadly interpret 'description' to mean an algorithm for computing z_n from n. We use the tools of computability theory to give negative answers to both questions.

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Randomized Push-Out Mechanism in Priority Queuing Systems

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Keywords. Priority queueing; preemptive priority; randomized push out mechanism.

Queuing system models are used everywhere in our life. There are many ways to complicate the simplest queuing systems models for making them look like the real ones. It can be done, for example by specialized push-out mechanism or prioritization.

The priority queuing approach allows to construct systems, where it is necessary to transfer data of varying importance. But using the systems with preemptive priority is significant only when the data streams have low intensities, because at the high-loaded system the effect of prioritization will be invisible due to the permanent system payload and consequently data loss. In the real life some systems have the flows with high intensity, for example computer networks. To solve this problem in the proposed model has been added specialised push-out mechanism, which allows pushing non-priority packets out of the system to free up the space.

In [1], Vilchevsky considers randomized push-out mechanism. This mechanism has one control parameter - the probability of pushing out "a", which can totally change the behavior of the queuing system. For example, when "a"$= 0$ system has no push-out mechanism, but when "a"$= 1$ system has an absolute one.

For studying such systems White, Christie and Stephan proposed to use a classical method of generating functions. It allows to obtain analytical expressions for the basic model characteristics. This paper presents the application results of this method to the systems with different priorities and randomized push-out mechanism. Also, the main characteristics of model depending on "a" were plotted. A change of the "a" parameter can effectively control the behavior of the priority system, even heavy-loaded, and significantly affect the characteristics of the model, without losing the prioritization of the data flows.

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The Fourier Basis of p-Adic Differentiable Functions

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Keywords. p-adic analysis; fractional differentiability; Fourier theory.

Let $\mathbb{Q}_p$ be the field of p-adic numbers, $\mathbf{K}$ a finite extension of $\mathbb{Q}_p$ of degree d, $\mathbf{o_K}$ its ring of integers and $\mathbb{C}_p$ its completed algebraic closure. Let $P_n(\Omega\cdot) : \mathbf{o_K} \to \mathbb{C}_p$ for $n \in \mathbb{N}$ be the Fourier basis of polynomial functions as constructed in [3].

Given a real number $r \geq 0$, we show in [1] that a function $f : \mathbf{o_K} \to \mathbb{C}_p$ is r-times differentiable (in the sense of [2]) if and only if $f(x) = \sum_{n\in\mathbb{N}} a_n P_n(\Omega x)$ with $|a_n| n^{rd} \to 0$ as $n \to \infty$.

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Analytical and Numerical Modelling of Nonlinear Vector Waves in a Chain Model of Anisotropic Crystals

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Keywords. Chain model; anisotropic crystal; bending mode; vector soliton.

Bending transverse waves in a nonlinear chain of particles is considered and a nonlinear vector equation for the phonon mode is derived. In the long-wave approximation the dispersion relation for such waves is: $\omega \sim k^2$. This dispersion law is typical for strongly anisotropic crystals [1]. The chain equation when each particle of number n is linked with two neighboring atoms from both sides reads:

$$m\frac{d^2\boldsymbol{\xi}_n}{dt^2} = \frac{T}{l}\left(\boldsymbol{\xi}_{n+1} - 2\boldsymbol{\xi}_n + \boldsymbol{\xi}_{n-1}\right) + \beta\frac{T}{2l}\left(\boldsymbol{\xi}_{n+2} - 2\boldsymbol{\xi}_n + \boldsymbol{\xi}_{n-2}\right) +$$

$$\frac{lK - T}{2l^3}\left[\left|\boldsymbol{\xi}_{n+1} - \boldsymbol{\xi}_n\right|^2\left(\boldsymbol{\xi}_{n+1} - \boldsymbol{\xi}_n\right) - \left|\boldsymbol{\xi}_n - \boldsymbol{\xi}_{n-1}\right|^2\left(\boldsymbol{\xi}_n - \boldsymbol{\xi}_{n-1}\right)\right] +$$

$$\beta\frac{2lK - T}{16l^3}\left[\left|\boldsymbol{\xi}_{n+2} - \boldsymbol{\xi}_n\right|^2\left(\boldsymbol{\xi}_{n+2} - \boldsymbol{\xi}_n\right) - \left|\boldsymbol{\xi}_n - \boldsymbol{\xi}_{n-2}\right|^2\left(\boldsymbol{\xi}_n - \boldsymbol{\xi}_{n-2}\right)\right],$$

where $\boldsymbol{\xi}_n$ is the particle displacement in the plane perpendicular to the chain, l is the distance between the atoms having masses m, T is the uniform tension of the chain, K is the analogue of Hook's constant, and β is the coupling constant. Similar equation but with $\beta = 0$ has been derived in [2] where coupling with only next neighboring particle was taken into consideration. In the long-wave approximation the derived equation with $\beta = -1/2$ can be reduced to the PDE:

$$\frac{\partial^2\boldsymbol{u}}{\partial t^2} + \frac{l^3T}{4m}\frac{\partial^4\boldsymbol{u}}{\partial x^4} + \frac{l^2K}{2m}\frac{\partial^2\left(|\boldsymbol{u}|^2\boldsymbol{u}\right)}{\partial x^2} = 0.$$

Solution properties of this equation are studied here in details both analytically and numerically. Among the solutions there are plane and helical nonlinear waves, both periodic and solitary.

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Using a Novel Methodology in Finding the Optimum Truss Structure

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Keywords. Optimization; space truss; artificial neural network.

Truss optimization has been an attractive area for researchers in recent years. Researchers are interested in this issue to find out how they can reduce the weight and cost while the structure satisfied with the physical constraints. To accomplish these requirements, trial and error method cannot be used because lots of trials will be required. Therefore, optimization methods should be used to find an optimum structure. In literature, Genetic Algorithm (GA), Simulated Annealing (SA), Harmony Search (HS) etc. are used in optimization of structures. Optimization methods mostly yield good results on determining design parameters. However, as the complexity of the space bar structure increases, the calculations become more difficult. To deal with this problem a methodology should be developed. This study aims to propose the desired methodology. Difficult calculations may be encountered in optimization of trusses, especially in complex space bar structures. Computers may not be sufficient to carry out the calculation of the optimization in some cases. In space bar structure, as the number of bar increases, the complexity of the bar space structure optimization increases. There is an exponential ratio between the number of bar and the optimization calculation. To avoid of the computational burden, a methodology will be proposed in this study. As a first step, structural analyses of the well-known example, 25 bar space truss, will be performed in finite element analysis software. The approximate model of the structural analysis will be obtained by using of Artificial Neural Network (ANN). The obtained approximate model will be used by Simulated Annealing for optimization of the structure. Therefore, it is expected that complex structures optimization will take shorter time to solve.

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On Solution Methods to Bilevel Problems with D.C. and Bilinear Goal Functions

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Keywords. Bilevel optimization; nonconvex problems; global search theory.

A hierarchy is one of the promising paradigm in mathematical programming in recent years [1]. In this work we investigate two classes of bilevel programming problems in an optimistic statement [2] :

$$F(x,y) \downarrow \min_{x,y}, x \in D, y \in Y_*(x), Y_*(x) \stackrel{\triangle}{=} \operatorname*{Argmin}_y \{G(x,y) \mid (x,y) \in D_1\}. \qquad (\mathcal{BP})$$

In the problems of the first class the upper level goal function is d.c. (represented by difference of two convex functions), and the lower level goal function is convex quadratic. In the problems of the second class the goal functions of the both levels are bilinear. The latter problems arise during the investigation of the problem of optimal pricing in telecommunication networks.

The new solution methods for these problems are elaborated. These methods based on a possibility of equivalent representation of a bilevel optimization problem as a nonconvex optimization problem [2] (with the help of Karush-Kuhn-Tucker conditions), and on the applying the Global Search Theory (GST) (for solving of the obtained nonconvex problem). Global Search Algorithms based on GST consist of two principal stages: 1) a special local search methods, which takes into account the structure of the problem under scrutiny [3]; 2) the procedures, based on Global Optimality Conditions [3], that allow to improve the point provided by the Local Search Method. Computational testing of the elaborated methods has shown the efficiency of the proposed approach.

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Mapping of the Graph of a Parallel Program to the Graph of a Computing System

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Keywords. Graph; quadratic assignment problem; genetic algorithm.

The goal of our research is to analyze the quadratic assignment problem that is a classic example of mapping linked objects in a discrete direction. In general, this problem is NP-hard. Researchers developed branch and bound method and heuristic methods to solve the above mentioned problem. Polynomial algorithms were developed for particular cases.

We investigate the case of weighted graphs mapping in which nodes represent objects and edges represent links. This problem can represent the process of mapping of a parallel task to a multiprocessor supercomputer to make the process of data transmission more efficient. In practice the size of such graphs may reach 100000 nodes per graph, consequently the use of exact algorithms for solving these types of problems is unreasonable.

For solving the assigned task we have proposed the heuristic genetic algorithm. We have developed a constructive operator which generates new solutions by copying the best characteristics of the parent solutions. Iterative algorithm for local optimization of solutions has been developed.

During our research we have conducted experiments on different classes of graphs and compared quality of solutions generated by our algorithm with the results obtained on the basis of other algorithms. The experiments showed that our algorithm works more efficiently on certain classes of graphs.

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Investigation of DIviding SIMPLices Algorithm for Symmetric Lipschitz Optimization Problems

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Keywords. Lipschitz optimization; global optimization; simplicial DIRECT-type algorithm; symmetric function.

In this talk, we consider a global optimization problem for a symmetric Lipschitz continuous function. Recently it was shown, that modification of the well-know DIRECT (DIviding RECTangles) algorithm by Jones et al. [2] adopted to solving symmetric Lipschitz continuous functions is efficient when it comes to solving such problems [1]. As symDIRECT uses hyper-rectangular partitions, the search space over-covers unique regions of symmetries. In such a case hyper-rectangles should be checked during optimization if they intersect the unique region in consideration. For symmetric optimization problems simplicial partitions are more suitable because simplicial unique regions may be formulated.

Simplicial partition based DISIMPL algorithm gives very competitive results to DIRECT for standard test functions and performs particularly well when the search space and the numbers of local and global optimizers may be reduced by avoiding symmetries [3]. The present talk is concerned with the application of DISIMPL algorithm to various symmetrical optimization problems: center-based clustering, nonlinear least squares regression, grillage-type foundations, etc. Based on the experiments, superiority of DISIMPL algorithm is shown: the number of function evaluations is significantly less than using symDIRECT.

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Assessing the Reliability of a Fully Coupled Eco-Hydrological Model Based on the Macroscopic Cellular Automata Approach

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Keywords. Macroscopic cellular automata; eco-hydrology; flow routing.

Macroscopic Cellular Automata (MCA), which represent an extension of the original computational paradigm of Cellular Automata, were used to develop a fully coupled eco-hydrological model. The latest version of the model adds a new module dealing with surface flow generation and routing to the existing three-dimensional unsaturated and saturated flow module, the soil-vegetation-atmosphere transfer scheme and the vegetation dynamics model.

Similarly to the unsaturated/saturated flow scheme, an analysis of the convergence of the discrete surface flux equation was carried out in order to assess the optimal time step for different configurations, in terms of cell dimensions and surface flow resistance coefficients (depending on land use). A careful analysis of the mass balance errors was also performed with the results achieved on a reference hillslope, having the same morphological characteristics of the Biosphere 2 hillslope experiment. Finally, results were validated with FLO-2D, a commercial flood routing model that simulates unconfined overland flow, highlighting the differences achieved when all the complex interactions between the soil-surface-atmosphere compartments are correctly modeled.

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Pattern Classification through Fuzzy Likelihood

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Keywords. Fuzzy; Bayes rule; classification; likelihood estimation

In the literature there are a lot of papers concerning fuzzy theory as a mean for classifying and extracting information from huge amount of data in a human-like fashion. Many authors have studied how to obtain a membership function of a fuzzy set by ad hoc heuristics, histograms, nearest-neighbor, etc. In [1] a definition of fuzzy likelihood measure was proposed in the similarity estimation context, while [2] put the basis of adaptive fuzzy likelihood algorithms in the context of system theory and fuzzy logic. In this paper, we start from the histograms of the observed data to obtain the membership function of a fuzzy set approximating the data distribution. The membership function is obtained combining together the raw data histogram with its successively smoothed versions. This membership function is in turn used to obtain a posterior probability through a suitable version of the Bayesian formula. It is important to note that since our likelihoods are fuzzy numbers a careful translation in terms of restricted fuzzy arithmetic has to be done for the classical Bayes rule in order to obtain meaningful probabilities.

To classify a member in a set we adopt the *overtaking* relation between fuzzy numbers introduced in [3]. The overtaking mimics an ordering relation between fuzzy numbers that depends on a assigned threshold delta. The ordering imposed by the overtaking relation translates immediately into a dominance of the posterior probability of a class over another for a given observed value. In this way a crisp classification is eventually obtained. The proposed method has been tested on a very standard data set: Fisher's Iris data set. The authors have implemented the proposed ideas in Matlab and performed classification over the three species using both one feature at each time or combining them using a naif Bayes approach. In all cases the results have been close to the theoretical optimal error rate.

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Gaussian Network Models for Protein Binding Site Comparison

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Keywords. Protein; binding site; alignment.

Accurately assessing the pairwise similarity of protein binding sites facilitates studies of protein function and evolution and aids in drug design. Accurate algorithms for binding site comparisons are particularly useful in drug repurposing – an emerging new approach in drug discovery which aims at finding new therapeutic indications for existing, FDA approved, drugs. While measuring structural similarity of rigid structural motifs is considered to be a solved problem, the existing structural similarity algorithms often fail to recognize structural homology of binding site motifs. This is largely due to proteins being flexible, dynamic molecules that are subject to conformational changes upon ligand binding.

We present a novel method for a structural motif comparison that utilizes a Gaussian Network Model (GNM) [1] to compute correlations between residue fluctuations and, in turn, to detect fragments corresponding to flexible binding site regions. Correlations between residue fluctuations are computed using nonzero eigenvalues and the corresponding eigenvectors of the Kirchhoff matrix of inter-residue contacts. An in-house structure comparison method, capable of finding a structural match of any upfront specified accuracy is then applied to separately align binding site fragments [2]. The final alignment and its score are computed by assembling the fragment alignments in either order-dependent or order-independent manner.

We use carefully designed benchmarking tests to demonstrate that our methodology compares favorably to existing algorithms for protein structure comparison.

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Stochastic Systems with Aftereffect and Methods of Their Numeric & Symbolic Solution

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Keywords. Stochastic system; delay; modeling.

A phenomenon of delays and hereditary effects is essential element of functioning of different frames, for example, control devices for technical processes, economic and social systems etc. Therefore functional differential equations (DE, FDE) including ordinary and partial deterministic and stochastic DE with divergent arguments (delay DE, neutral delay DE) and integro-differential equations (IDE) are of particular interest both from theoretical and practical viewpoints. As it is well-known, methods for analysis of such systems are very complicated [1].

The main part of our schemes to study the systems is based on a combination of the classical method of steps and an extension of the phase space [2,3]. The aim of the apparatus is to transform a source non-Markovian vector process into a Markovian one and to obtain a chain of simple solvable tasks instead of one compound problem. All our developments for stochastic FDE considered are based on the unified combination and allow to calculate the main probabilistic characteristics of unknown random state vectors.

We apply our schemes for study of linear and nonlinear FDE with single and multiple, constant and variable delays, systems excited by continuous and discrete fluctuations, with additive and multiplicative noises, estimation of stochastic sensitivity for linear dynamic systems with delay etc.

In addition, our technique coupled with the Monte Carlo method can be used to solve very complicated nonlinear stochastic problems.

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Domain Decomposition Multigrid Methods for the Numerical Solution of Parabolic Equations

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Keywords. Domain decomposition; multigrid; parabolic equation.

In this work, we propose efficient discretizations for unsteady diffusion problems that suitably combine non-iterative domain decomposition techniques and geometric multigrid methods. The spatial domain is considered to be discretized via a semi-structured triangular grid. To this end, an unstructured coarse triangulation $\mathcal{T}_H$ is first constructed and its elements are subsequently refined using regular triangular meshes. The resulting fine triangulation is conforming and will be denoted by $\mathcal{T}_h$.

In this context, we consider a finite element spatial discretization in combination with a time splitting scheme. In particular, we define a three-component splitting formula (cf. [1]) related to a decomposition of the fine triangulation $\mathcal{T}_h$ into three sets of nodes: a) those lying strictly inside the elements of $\mathcal{T}_H$; b) the vertices of $\mathcal{T}_H$ and its neighbouring nodes in $\mathcal{T}_h$; and c) the rest of the nodes (all of them lying on the edges of $\mathcal{T}_H$). As a result, the equations corresponding to the first set of nodes decouple across the elements of $\mathcal{T}_H$ and will be solved in parallel using geometric multigrid techniques (cf. [2]).

The method is unconditionally stable and computationally efficient, since it avoids the need for Schwarz-type iteration procedures. Furthermore, it extends the ideas discussed in [3] for rectangular elements to the case of triangular grids, thus yielding much more flexibility in the discretization of complex domains. The practical utility of the algorithm is illustrated by a collection of numerical experiments.

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A Deterministic Algorithm for Multi-Objective Constrained Optimization

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Keywords. Multiobjective constrained optimization.

In this paper, we are concerned with finding a set of optimal trade-offs, the so-called Pareto-optimal set for constrained multiobjective optimization programs. Many numerical methods for constructing Pareto-set approximations have been proposed so far. Most of them are heuristic, i.e. they dont guarantee the optimality of the found solutions. We formally define notion of an approximate solution — ε, δ-Pareto set and prove some important properties of this set. We propose a deterministic algorithm to construct finite ε, δ-Pareto set. The algorithm is based on non-uniform space covering techniques [1, 2]. Its convergence in a final number of steps is formally proved. The serial and parallel implementations of the algorithm are discussed. The proposed approach is experimentally compared with some other well-known approaches to constructing Pareto-frontier approximations.

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Resource Allocation within the Controlled Hierarchical Systems

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Keywords. Controlled hierarchical systems; resource allocation.

The resource allocating hierarchical system is modelled with a connected loop- and circuit-free graph $G = (V, A)$, $A \subseteq V^2$, with the nodes V which define the elements of the system, and the arcs A, defining the element connections. Let V^a, V^p be the separation of the set V; $V^{inl} = \{i|(j,i) \bigcap A = \oslash,\ j \in V\}$, $V^{out} = \{i|(i,j) \bigcap A = \oslash,\ j \in V\}$, $V^{inl} \subseteq V$, $V^{out} \subseteq V$; $K(\nu) = \{i|(i,\nu) \in A,\ i \in V\}$, $\nu \in V$; I be the weights set (or resources characteristics) of graph nodes. The system receive the controls, defined by the set denoted as U^ν, $\nu \in V^a$. Lets denote characteristics vector on ν-th element inlet as $\overrightarrow{w}^\nu$, $\nu \in V$, $\overrightarrow{w}^\nu \in R^{|I|}$; minimal and maximal values of i-th characteristic on ν-th element's inlet as W_i^ν and Q_i^ν, minimal and maximal values of i-th characteristic on ν-th element's outlet as H_i^ν and S_i^ν, $\nu \in V$; the function transforming ν-th element's inlet characteristics to outlet ones as $\overrightarrow{\varphi}^\nu(\overrightarrow{w}^\nu, \overrightarrow{u}^s, \delta) \in R^{|I|}$, $i \in I$, $\nu \in V$; parameter which equals to 1, if $\nu \in V^a$, and equals to 0 if $\nu \in V^p$, $\overrightarrow{u}^s \in U^\nu$, $\nu \in V$ as δ; the vector-function defining ν-th element inlet characteristics using the outlet characteristics of all the elements straight preceding to element ν as $\overrightarrow{f}^\nu(\overrightarrow{\varphi}^\nu(\overrightarrow{w}^\nu, \overrightarrow{u}^s, \delta))$, $s \in K(\nu)$, $\nu \in V$; the function of ν-th element's expenses under control $\overrightarrow{u}^\nu$ as $\overrightarrow{\phi}^\nu(\overrightarrow{w}^\nu, \overrightarrow{u}^s)$, $\nu \in V^a$; the known characteristic values for elements $\nu \in V^{inl}$ as $\overrightarrow{q}^\nu$, and the required characteristic values for elements $\nu \in V^{out}$ as $\overrightarrow{g}^\nu$, $\overrightarrow{q}^\nu \in R^{|I|}$, $\overrightarrow{g}^\nu \in R^{|I|}$. The problem is to find the values of $\overrightarrow{w}^\nu$, $\nu \in V$, and $\overrightarrow{u}^s$, $\overrightarrow{u}^s \in U^\nu$, $\nu \in V^a$ for which the following conditions are true:
$W_i^\nu \le w_i^\nu \le Q_i^\nu$, $i \in I$, $\nu \in V$; $H_i^\nu \le \overrightarrow{\varphi}^\nu(\overrightarrow{w}^\nu, \overrightarrow{u}^s, 0) \le S_i^\nu, i \in I$, $\nu \in V^p$; $H_i^\nu \le \overrightarrow{\varphi}^\nu(\overrightarrow{w}^\nu, \overrightarrow{u}^s, 1) \le S_i^\nu, i \in I$, $\nu \in V^a$; $\overrightarrow{w}^\nu = \overrightarrow{q}^\nu, \nu \in V^{inl}$; $\overrightarrow{\varphi}^\nu(\overrightarrow{w}^\nu, \overrightarrow{u}^s, 0) = \overrightarrow{g}^\nu$, $\nu \in (V^{out} \bigcap V^p)$; $\overrightarrow{\varphi}^\nu(\overrightarrow{w}^\nu, \overrightarrow{u}^s, 1) = \overrightarrow{g}^\nu$, $\nu \in (V^{out} \bigcap V^a)$; $\overrightarrow{w}^\nu = \overrightarrow{f}^\nu(\overrightarrow{\varphi}^\nu(\overrightarrow{w}^\nu, \overrightarrow{u}^s, 0))$, $s \in K(\nu)$, $\nu \in (V^p \backslash V^{inl})$; $\overrightarrow{w}^\nu = \overrightarrow{f}^\nu(\overrightarrow{\varphi}^\nu(\overrightarrow{w}^\nu, \overrightarrow{u}^s, 1))$, $s \in K(\nu)$, $\nu \in (V^a \backslash V^{inl})$, and moreover the value of $\sum_{\nu \in V^a} \overrightarrow{\phi}^\nu(\overrightarrow{w}^\nu, \overrightarrow{u}^s)$, is minimal.
Within the frames of developed mathematical model there is possible to state the optimization problems of gas transport systems parameters calculation, of multi-mode equipment industry systems scheduling, of heat supply systems optimal modes finding.

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Syntactic – Semantic Axiomatic Theories in Mathematics

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A more careful consideration of the recently introduced "Grossone Theory" of Yaroslav Sergeyev [1], leads to a considerable enlargement of what can constitute possible legitimate mathematical theories by the introduction here of what we may call the *Syntactic – Semantic Axiomatic Theories in Mathematics*. The usual theories of mathematics, ever since the ancient times of Euclid, are in fact axiomatic, [1], which means that they are *syntactic* logical consequences of certain assumed axioms. In these usual mathematical theories *semantics* can only play an *indirect* role which is restricted to the inspiration and motivation that may lead to the formulation of axioms, definitions, and of the proofs of theorems. In a significant contradistinction to that, and as manifestly inspired and motivated by the mentioned Grossone Theory, here a *direct* involvement of *semantics* in the construction of axiomatic mathematical theories is presented, an involvement which gives semantics the possibility to act explicitly, effectively, and altogether directly upon the usual syntactic process of constructing the logical consequences of axioms. Two immediate objections to what appears to be an unprecedented and massive expansion of what may now become legitimate mathematical theories given by the *syntactic – semantic axiomatic theories* introduced here can be the following: the mentioned direct role of semantics may, willingly or not, introduce in mathematical theories one, or both of the "eternal taboo-s" of *inconsistency* and *self-reference*. Fortunately however, such concerns can be alleviated due to recent developments in both inconsistent and self-referential mathematics, [2–3]. Grateful recognition is acknowledged here for long and most useful ongoing related discussions with Yaroslav Sergeyev.

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Complete Solutions to Nonconvex Fractional Programming Problems

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Keywords. Nonconvex fractional program; sum-of-ratios; global optimization; canonical duality.

Fractional programming problem belongs to a class of sum of ratios problems that have been actively studied for several decades. Depending on the nature of each application, the function can be affine, convex or concave. However, even for the simplest case in which all functions are all affine functions, the problem is still a global optimization problem that may have multiple local optima. Based on the properties of problem, the speaker will explain how to relax the fractional structure by introducing a family of paramedic sub problems. And the canonical dual of each sub problem becomes a concave maximization problem that exhibits no duality gap. Since the infimum of the optima of the parameterized sub problems leads to a solution to the original problem, then the optimality conditions and existence conditions for finding a global minimizer of the original problem are provided. The talk concludes by pointing out some recent algorithms.

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Spatial Prisoner's Dilemma for Socio-Economic Dynamics

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Keywords. Prisoner's dilemma; cellular automata; reciprocity.

Evolutionary games represent a basic tool for modeling socio-economic dynamics. Relations of reciprocity were explored through the Repeated Prisoner's Dilemma (RPD) by L. Bruni [1] for analyzing some aspects of the gratuity, as an extreme form of cooperation.

In this work, such questions were reconsidered by RPD extension to a spatial context using the Cellular Automata (CA) approach of Nowak [2] by stochastic spatial distribution of agents and adoption of different strategies.

Each cell of a finite two-dimensions Cellular Automaton with square cells is occupied by one agent owning a RPD strategy. The agent relates with all the agents in adjacent cells in terms of RPD. Our model [3] introduces new behaviors of agents through altering payoffs and symmetry.

Results show that the spatial RPD converges more rapidly to almost total cooperation or defection in comparison with simple RPD, but some values of payoff generate an interesting chaotic evolution of the system. Furthermore unexpected results concern the emergence of cooperative behaviors in agents with complex strategies, in spite of their reduced conditions of increasing own payoff.

Such a model can be improved from this primitive version toward a more sophisticated one in order to permit a comparison between some simple real situation and its simulation by spatial RPD.

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A Provably Tight Delay-Driven Concurrently Congestion Mitigating Global Routing Algorithm

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Keywords. Steiner tree; global routing; Elmore delay; gradient method.

Routing is a very important step in VLSI physical design. A set of nets are routed under delay and resource constraints in multi-net global routing. Here a delay-driven congestion-aware global routing algorithm [1] is developed, which is a heuristic based method to solve a multi-objective NP-hard optimization problem. The proposed delay-driven Steiner tree construction method is of $O(n^2 \log n)$ complexity, where n is the number of terminal points and it provides n-approximation solution of the problem for a certain class of grid graphs. The existing timing-driven method [2] has a complexity $O(n^4)$ and is implemented on very small number of nets. Next we propose an $(1+\epsilon)$–approximation gradient algorithm for minimizing the overflow. This is a concurrent approach considering all the nets simultaneously contrary to the existing approaches of sequential rip-up and reroute. The algorithms are implemented on ISPD98 derived benchmarks and the drastic reduction of overflow is observed.

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The Lower Bound of Changes in Production Operations

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Keywords. Convex programming; active constraints; number of changes.

A relationship between two tasks of manufacturing process planning with an unstable (fluctuating) supply of raw materials is considered.

The first task (the optimization of streamlining manufacturing operations) is stated [1] as a problem of convex programming: find a vector $X^0 \in D$, which minimizes the function: $F(X) = \sum_{i=1}^{n} f(x_i)$, where $f(x_i)$ is a convex function and D is a special set of R^n with lower and upper constraints:

$$D = \{X \in R^n : A_j \leq \sum_{i=1}^{j} x_i \leq B_j, j = \overline{1, n-1}, \sum_{i=1}^{n} x_i = B_n\}$$

.

The second task is to find a vector $X^* \in D$ with the least number of changes, such as, $i \in \{1, 2, ..., n-1\}$, where $x_i^* \neq x_{i+1}^*$.

The optimal vector X^0 might be found by means of the active inequality constraints of the set D. Generally, a set of p active constraints consists of number $q, (q \leq p)$ groups of the same (either lower or upper) type's constraints. It is shown [1] that in the particular case when $q = p$ the optimal vector X^0 coincides with one of the vectors X^* (as a rule, there is a set of these vectors).

Otherwise, let $M_{j_k}, k = \overline{1, q}, j_k < j_{k+1}$, be representatives of these groups, and

$$y_k = \frac{M_{j_k} - M_{j_{k-1}}}{j_k - j_{k-1}}, k = \overline{1, q+1}(j_0 = 0, M_{j_0} = 0, j_{q+1} = n, M_{j_{q+1}} = B_n).$$

Theorem. Let every pair of the values y_k and $y_{k+1}, k = \overline{1, q}$, fit the inequality of $y_m < y_{m+1}$ $(y_m > y_{m+1})$, if the active constraint M_{j_k} is upper (lower) constraint. Then q will be the least possible number of changes for any $X \in D$.

The algorithm of plans calculation having minimal number of changes is elaborated and applied to solve some test problems.

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Numerical Analysis of the Radiating Fins Used in Solar Cell Concentrators

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Keywords. Monte Carlo methods; nonlinear Poisson equation; multigrid methods.

In this study we analyzed the fin efficiency of the space radiator placed in a Cassegrain type solar cell concentrator system. Solar cell concentrator systems have two distinct advantages over the at panel systems. First, concentrated light increases the efficiency of the solar cells. Secondly, solar cell concentrator system provides shielding against charged particle radiation and micro particles. But solar cells convert only some part of the the reflected light to the electrical energy. Rest of the light energy is converted to the heat. A space radiator is required to transfer excessive heat into space via radiation. If concentrated light energy reflected on the solar cell is not removed and radiated into space, the solar cell becomes very hot and get damaged. The excessive heat should be carried to a larger radiation area and the operating temperature of the solar cell should be lowered. The dimensions, emittance and the temperature distribution on the radiating fin will provide operating temperature of the solar cell under the concentrated light. We calculated the temperature distribution of the fin using finite-difference scheme. This 2-dimensional nonlinear conduction-radiation problem is solved using both Monte Carlo and Multigrid methods. Both methods are compared according to their solution efficiency and accuracy. Following operating temperature of the solar cell is calculated and fin dimensions are optimized for a safe solar cell temperature.

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Numerical Infinitesimals for Solving ODEs

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Keywords. Numerical infinitesimals and infinities; ordinary differential equations; Infinity Computer; Taylor expansion; automatic control of rounding errors.

There exists a huge number of numerical methods (see, e.g., [1] and references given therein) that iteratively construct approximations to the solution $y(x)$ of an ordinary differential equation (ODE) $y'(x) = f(x, y)$ starting from an initial value $y_0 = y(x_0)$ and using a finite approximation step h that influences the accuracy of the obtained approximation. In this talk, a new computational methodology (see [2, 3]) is used for solving ODEs on a new kind of a computational device – the Infinity Computer (its working prototype exists). The new computer is able to work numerically with finite, infinite, and infinitesimal quantities giving so the possibility to use different infinitesimals numerically and, in particular, to take advantage of infinitesimal values of the approximation step h.

Since very often in scientific and technical applications it happens that the person who wants to solve an ODE is not the person who has written the code for $f(x, y)$, it is supposed that the person solving the said ODE does not know the structure of $f(x, y)$, i.e., it is a 'black box' for him/her. Under this condition, it is proved that the Infinity Computer is able to calculate derivatives of the solution $y(x)$ and to reconstruct its Taylor expansion of a desired order numerically. It should be stressed that this can be done without finding the respective derivatives analytically (or symbolically) by the successive derivation of the ODE, as it is usually done when the Taylor method is applied.

Methods using approximations of derivatives obtained thanks to the usage of numerical infinitesimals are also discussed and a technique for an automatic control of rounding errors is introduced. Numerical illustrations are given.

Acknowledgements.

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Hybrid High-Precision Supercomputer Systems

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Keywords. Hybrid supercomputer system; Grossone numeral; functional programming language.

The talk presents a project proposed by the authors to create a hybrid supercomputer system for high-precision calculations using the new computational methodology and data representation format based on the Grossone numeral [1].

As a computing system hardware we propose to use a polymorphic architecture that includes traditional central processor units, specialized graphics accelerators and computing based on FPGA integrated circuits. The usage of the heterogeneous hardware platform optimizes the performance of the calculator while using complex data types and a positional notation for operating with infinitesimal and infinite quantities by using the Grossone numeral system.

At the software level of the considered system it is planned to implement new interface solutions and language tools for constructing algorithms that significantly facilitate encoding operations with complex mathematical objects, not necessarily having a numerical nature and the development of efficient computational methods in the case of non-smooth and multiextremal problems, including those with non-convex constraints, by using, in particular, the dimension reduction approaches based on new fractal mapping techniques.

One of the key elements of the new computing system is the usage of functional programming language *Refal* that is widely used for a number of applications, including the implementation of high-precision calculations in astronomy and the task of data mining, as well as the solution of the translational tasks when creating high-level language compilers for the new computing models of different types.

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Inverse Problems for Nonlinear Schrödinger Operator

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Keywords. Nonlinear Schrödinger; Born approximation; inverse problem.

This work deals with the nonlinear Schrödinger equation

$$-\Delta u + h(x,|u|)u = k^2 u, \quad x \in R^n, \quad n = 2,3,$$

where h denotes the index of refraction in general form.

This equation appears quite naturally in applications. It includes the linear case and the basic nonlinearities which can be met in nonlinear optics.

In the scattering theory one considers the scattering solutions, that is the solutions of the form

$$u(x,k,\theta) = u_0(x,k,\theta) + u_{sc}(x,k,\theta),$$

where $u_0(x,k,\theta) = e^{ik(x,\theta)}$ is the incident plane wave with direction $\theta \in S^{n-1}$-unite sphere, and $u_{sc}(x,k,\theta)$ is the scattered wave. In inverse scattering problems we are asked to extract information about h from the knowledge of the scattered wave at large distances, i.e., from the so-called scattering amplitude $A(k,\theta',\theta)$.

We prove an analog of the well-known Saito's formula for this nonlinear Schrödinger operator

$$\lim_{k\to+\infty} k^{n-1} \int\limits_{S^{n-1}\times S^{n-1}} e^{-ik(\theta'-\theta,x)} A(k,\theta',\theta)\, d\theta\, d\theta' = \frac{(2\pi)^n}{\pi} \int\limits_{R^n} \frac{h_0(y)}{|x-y|^{n-1}}\, dy,$$

where $h_0(y) := h(y,1)$. This formula allows us to prove the uniqueness theorem for reconstruction of h_0.

The properties of the scattered wave and the definition of the scattering amplitude allow us to introduce the inverse Born approximation q_B as

$$q_B(x) := F^{-1}(A(k,\theta',\theta))(x).$$

Next we study the following problem: To estimate the smoothness of the terms from the Born approximation. For h_0 from $L^p_{loc}(R^n)$ the main result is:

$$q_B(x) - h_0(x) \in H^t_{loc}(R^n).$$

Fixed energy problem for nonlinear Schrödinger equation is also considered.

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A New Method Improving the Convergence Performance of IRWLS-Based All-Pass IIR Filters

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Keywords. L_∞ (minimax norm); weighted least squares; all-pass IIR filters.

We consider the design problems that affect equiripple all-pass IIR filters. First, we describe a method of solving the phase error minimization problem for the phase of a filter and the desired phase. We utilize a method that involves linearizing a nonlinear optimization problem and then solving the filter design problem in the same manner as the conventional method. Next, we describe the norm which is a measure of the phase error. The L_2 norm and L_∞ (minimax norm) are often used as the values for the norm in a phase-error minimization problems. When using the L_∞ norm, this is known as the equiripple design method, and many similar design methods have been proposed [1, 3, 4]. In particular, the iteratively reweighted least squares (IRWLS) method, based on a scheme that involves multiplying a least square error by a weighting function , is a typical equiripple design method [2–4]. However, the convergence performances of the relevant solutions have not been referred to in these papers. Moreover, there are even cases where the convergence of a solution becomes unstable in some design examples. In order to overcome these instability problems in terms of solution convergence, we introduce a new weighting function that can be used in the IRWLS method. We show experimentally how introducing the weight function into some design examples that did not originally result in convergence when using the conventional method improves the convergence performance in the solution of the IRWLS.

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Range Reduction Method for Generating Random Vectors

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Keywords. Random number generation; random vector; algorithm.

We consider an important and complicated problem of generating continuous multi-dimensional random variables or random vectors. Most universal methods of generating random vectors (i.e. methods that can be implemented for a wide class of distributions and do not exploit specific properties of certain distributions) belong to two main classes: Markov chain methods and acceptance-rejection methods. We assert that a new universal method based on an approach alternative to the approach of the above-mentioned classes can be effectively implemented for generating random vectors. This method, which was named the range reduction (RR) method, was presented in [1]. It was proposed and described as a method for generating one-dimensional discrete random variables. In this work we prove that this method extends to the case where the generated variable is continuous and multi-dimensional. Here we present the general version of the RR algorithm which enables one to implement it for generating random vectors. We consider a random vector X with probability density function (pdf) $f(\overrightarrow{x})$ whose range (set of points where the pdf is positive) is designated as R_x. The RR algorithm for generating X requires the choice of an instrumental random vector Y such that an efficient algorithm for its generation exists. The pdf of Y is designated as $g(\overrightarrow{x})$.

In order to describe the algorithm we introduce the following notations. Let D designate the random vector whose pdf $d(\overrightarrow{x})$ takes positive values $(f(\overrightarrow{x})-g(\overrightarrow{x}))/I$ in $R_f = \{\overrightarrow{x} \in R_x : f(\overrightarrow{x}) > g(\overrightarrow{x})\}$. Here I designates the integral $\int_{R_f}(f(\overrightarrow{x})-g(\overrightarrow{x}))d\overrightarrow{x}$. Let XRND, YRND, DRND designate the generated values of X, Y, D respectively. The algorithm includes the following steps.

1. Generate Y.

2. Generate U uniformly distributed in (0,1) independent of Y.

3. If $URND \leq f(YRND)/g(YRND)$, set XRND=YRND; otherwise generate D and set XRND=DRND.

The validity of the RR method is proved, its performance examined, and examples illustrating the advantages of the method are given.

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Solving Max-Cut Problem via Global Equilibrium Search

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Keywords. Max-cut; global equilibrium search.

The maximum cut problem is a well-known NP-hard problem, which recently gathered a lot interest due to a number of important practical applications [1,2]. The input for the maximum cut problem is an undirected graph $G = G(V, E)$, where each edge $(i, j) \in E$ is assigned a certain weight w_{ij}. Let (V_1, V_2) be a partition of the set of vertices V into two disjoint subsets. A cut (V_1, V_2) in G is any subset of edges $(i, j) \in E$, such that $i \in V_1$ and $j \in V_2$. The maximum cut problem consists in finding a cut in graph G with the maximum sum of the edge weights.

We consider an extension of the algorithm for the maximum cut problem based on global equilibrium search (GES) discussed in [3]. The comparison with other available algorithms using a set of 74 benchmark problems revealed that GES dominates other approaches in terms of computational speed and solution quality. The implementation of GES presented in [4] maintains a set of solutions, which are used to prevent algorithm from converging to previously visited areas in the search space. Since this set contains high quality solutions, it is desirable to use it in a more efficient manner. Assuming that high quality solutions share some common structure, one can try to combine their components in an attempt to find an enhanced solution. As a result, records have been improved for the 37 test problems, for others 36 known records found.

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Towards a New Philosophy of Mathematics Starting from Grossone Methodology

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Keywords. Philosophy of mathematics; Grossone approach to infinity; numbers and numerals.

Recently a new methodology for executing numerical computations with infinite and infinitesimal quantities has been introduced in [1,2]. This approach proposes a new counting system based on an infinite unit of measure – grossone. The methodology formulates three postulates that lead to a new promising philosophy of mathematics having a strong applied character. This approach has already attracted attention of philosophers (see [3, 4] and references given there).

The goal of this talk is to discuss general postulates of this new direction in Philosophy of Mathematics, to analyze its interrelations with other positions, and to study its possible origins. One of the key points of the new approach is to separate the mathematical objects under the observation and mathematical tools used for this observation (for example, a number is an object, and a numeral is an instrument). This and others peculiarities of the new philosophy of mathematics are discussed in detail in the talk.

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New Numerical Technique for Solving Two Dimensional Burgers' Equations Based on Similarity Reductions

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Keywords. Two dimensional Burgers' equations; finite difference method; local similarity solutions.

Central finite-difference approximations for solutions of the two dimensional Burgers' equations lose diagonal dominance at high cell Reynolds numbers. The popular remedies for this problem are the upwind differencing schemes. These schemes suffer from the accuracy deterioration near to the boundaries because of their enlarged differencing stencils. In this study, we developed a new scheme which is diagonally dominant at all cell Reynolds numbers for solutions of the two dimensional Burgers' equations. This scheme is based on similarity reductions of the two-dimensional Burgers' equations on small sub-domains defined by the classical five-point stencil. The resulting similarity equations, with similarity parameters in time and one spatial direction, are integrated analytically. The analytical solutions are then used to approximate the flux vectors in the two-dimensional Burgers' equations leading to diagonally dominant scheme at all cell Reynolds numbers. The scheme is derived here to demonstrate the approach. Numerical results are obtained for test problems. The computed results using our scheme confirm the developments of the present approach.

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A Purposive Sampling Method for Lava Flow Susceptibility at Mount Etna (Italy)

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Keywords. Non-uniform Grids; lava susceptibility; Etna.

In this study, a new method based on purposive sampling and on a non-uniform grid of sources, coupled with the numerical simulation of independent events, has been considered to evaluate the hazard induced by flow-type phenomena, and applied to lava-flows at Mt. Etna (Italy). The method aims at refining the spatial distribution of hypothetical eruptive vents with respect to an original uniform grid. The employed model is SCIARA-fv2, a Cellular Automata numerical model recently applied to the same study area for preliminary hazard analyses. The set of the whole performed simulations has been analysed into a GIS environment, to verify the number of events affecting each cell of the domain. In this way, lava-flow susceptibility could be evaluated in relative terms, by normalizing the number of affecting flows to the total number of simulations. On the basis of historical data, a reduced number of sampled eruptions with respect to previous exhaustive experiments was considered on the area, giving rise to an output representing the expected "scenario" in the next 100 years, which could be effectively used for either planning or civil protection purposes.

With respect to a uniform distribution of vents, the non-uniform one allows to map lava flows erupted from highest-probability sources with a finer resolution, thus significantly improving the reliability of the susceptibility map. Eventually, the same method could also be applied to evaluating the hazard induced by other types of flow phenomena, such as debris flows and avalanches.

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Modern Methods for Solving Problems with Hidden Nonconvex Structures

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Keywords. Nonconvex optimization; d.c. functions; global search methods.

A huge of optimization problems arising from different application areas are nonconvex. Meanwhile, there are even more real-life problems in which it is rather difficult to discover a nonconvex structure in the beginning of investigation. Consider, for example, the problems, that have been formulated as principal objectives for Mathematical Optimization Society in XXI century [1]: A) numerical search for equilibria; B) hierarchical problems; C) complementarity problems and variational inequalities; D) dynamical optimization. So a new mathematical apparatus is needed, this one that expands our abilities to find namely a global solution in real-life nonconvex problems, in particular, providing a possibility to escape critical (stationary) points and local solutions.

We consider optimization problems with (d.c.) functions of A. D. Alexandrov, representable as the difference of two convex functions. As known, this class forms the linear space with very nice properties [3]. We develop the Global Search Theory consisting of the following parts: I) the family of local search methods special for each kind of nonconvex problems (d.c. minimization, reverse-convex problems etc.); II) the family of Global Optimality Conditions (GOC); III) procedures of escaping local pits based on GOC; IV) global search methods based on GOC; V) convergence theorems for methods from I) and IV). Note, that the new technology opens the door for application of convex optimization methods [2] in nonconvex optimization. Applying this technology we were successful to solve some problems of kind A) search for Nash equilibria in the bimatrix game, B) bilevel problems with quadratic-linear data, C) linear complementarity problems with an indefinite matrix, D) nonconvex optimal control problems.

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Development of the Method of Computer Analogy for Analyzing and Solving Complex Systems

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Keywords. Computer analogy; differential equations; nonlinear systems.

We consider the classical computer with general properties as a device which solves problems using numerical approximation. The philosophical aspects of this issue are discussed, namely, how analytical operations correlate with operations of the computer. On this ground, we construct a mathematical model of the ideal digital computer and tend to reduce a large amount of operations in opposition to the classical computer which has to perform each operation. We optimize calculations or in some cases provide an explicit approximation of the solution. The computer analogy implies that we follow the same principles that are used in calculations in the computers: 1) numbers are represented by the segments of a power series; 2) there is a procedure of digit shifting. The value of the unknown function is represented as a segment of the power series in powers of a step τ of the independent variable. The finite difference methods can then be put into the proposed mathematical framework. The process of computation in this model can be effectively studied and improved. We found that the senior digits exhibit stochastic behaviour and thus can be averaged by the means of the probabilistic analysis. In terms of the numerical solution, this leads to excluding intermediate computations in the recurrent formula. This method can provide a solution in the explicit form. The final analytical solution is treated as the limit when τ tends to zero. If the full solution is difficult to obtain, then the method of computer analogy can be used for constructing simple asymptotic approximations. In [1] we applied the proposed method to solve nonlinear differential equations and systems, in the present paper we examine and solve more complex systems such as the systems of kinetic equations and the Lorenz system, etc. Periodic behaviour of the solution is investigated by studying the digit shifting process.

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Curvilinear Search and Higher Order Methods

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Keywords. Unconstrained optimization; higher order methods; curvilinear search.

The Halley class of methods is a class of higher order methods. Methods in this class are under suitable assumptions locally convergent and have a third order rate of convergence. The Halley class contains well known methods, such as Chebyshev, Halley and super-Halley methods. The Halley class can be written as a two-stage methods where the new iterate is updated by a combination of the current point and two directions; the Newton direction and a correction direction using the third derivative.

Curvilinear search is a global strategy that searches along a curve defined by two directions using backtracking. The two most used directions in unconstrained optimization are defined by a descent direction and a direction of negative curvature. The descent direction is utilizing a modified factorization of the Hessian matrix to guarantee descent and stability. Rarely, a curvilinear search uses a direction based on third order derivatives.

In this talk, we present an algorithmic framework for solving unconstrained optimization problems. It is based on introducing the curvilinear search as a combination of Newton's direction and a direction uses tensor/higher order derivatives of the objective function. We show under standard assumptions that the Halley class combined with a curvilinear search is globally convergent. In addition, limit points of the sequence of iterates will be stationary points. Under suitable choices of the directions the Hessian matrix at the limit points will be positive semidefinite. Moreover, if the Hessian at the limit-point is positive definite then the sequence of iterates converges with Q-cubic rate of convergence. We also provide numerical experiments on test problems from the MINPACK and CUTE collections which illustrate the theoretical findings.

Worst Case Computation Time for Minimal Joint Hamming Weight Numeral Systems

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Keywords. Numbers and numeral systems; minimal joint Hamming weight; graph algorithms.

In this talk, we analyze the worst case computation time using redundant numeral systems on multi-scalar multiplication, which is one of the bottle-neck operation of elliptic curve cryptography. The operation is to compute $S = \sum_{i=1}^{d} r_i P_i$ when $r_i \in \mathbb{Z}^+$ and P_i are points on elliptic curve. The computation time is strongly associated with the joint Hamming weight of the numeral systems. Most of previous works in this subject have focused on the average joint Hamming weight of each system [1]. However, having a different computation time for each input is prone to be weak against side channel attack, and we need to put dummy operations to make the computation time for all input to be as slow as the time for the worst case [2].

In this work, we propose a method for finding the largest joint Hamming weight for $\langle r_i \rangle_{i=1}^{d} \in \mathbb{Z}_{2^n}^d$ and digit set $D_S = \{0, \pm 1, \pm 3, \ldots, \pm(2h+1)\}$. We propose a graph algorithm for finding a circle C such that $\sum_{e \in C} \frac{w_e}{||C||} \geq \sum_{e \in C'} \frac{w_e}{||C'||}$ for any circle C' in the same graph, and apply the algorithm to our AJHW Markov chain [1]. As a result, we can analyze the worst computation time for several numeral systems. We found the value for $h \leq 513$ when $d = 1$, for $h \leq 9$ when $d = 2$, and for $h = 1$ when $d = 3, 4$. This matches the results by Muir [3] when $d = 1$ and the result by Solinas [4] when $d = 2, h = 1$.

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Convergence of a Family of Discrete Distributed Elliptic Optimal Control Problems with Respect to a Parameter

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Keywords. Distributed optimal control problems; numerical analysis; convergence with respect to a parameter.

We consider a bounded domain Ω in R^n whose regular boundary $\partial\Omega$ consists of the union of two disjoint portions Γ_1 and Γ_2 with $meas(\Gamma_1) > 0$ and $meas(\Gamma_2) > 0$. The convergence of a family of continuous distributed optimal control problems P_α, governed by elliptic variational equalities, when the parameter α of the family (the heat transfer coefficient on the portion of the boundary Γ_1) goes to infinity was studied in [2]. It has been proved that the optimal control, and their corresponding system and adjoint states are strongly convergent, in adequate functional spaces, to the optimal control, and the system and adjoint states of another distributed optimal control problem P governed also by another elliptic variational equality with a different boundary condition on the portion of the boundary Γ_1.

We consider the discrete approximations $P_{h\alpha}$ and P_h of the optimal control problems P_α and P respectively, for each $h > 0$ and for each $\alpha > 0$, through the finite element method with Lagrange's triangles of type 1 with parameter h (the longest side of the triangles). We also discrete the elliptic variational equalities which define the systems and their adjoint states, and the corresponding cost functional of the optimal control problems P_α and P [1]. The goal of this paper is to study the convergence of this family of discrete distributed elliptic optimal control problems $P_{h\alpha}$ when the parameter α goes to infinity. We prove the convergence of the discrete optimal controls, the discrete system and adjoint states of the family $P_{h\alpha}$ to the corresponding to the discrete optimal control problem P_h when $\alpha \to +\infty$, for each $h > 0$, in adequate functional spaces.

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On the Numerical Solution of Some Nonlinear and Nonlocal Boundary Value Problems

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Keywords. Boundary value problem; numerical method; fixed point.

The modeling of various physical questions in plasma kinetics and heat conduction lead to nonlinear boundary value problems involving a nonlocal operator, such as the integral of the unknown solution, which depends on the entire function in the domain rather than at a single point. Recently, the nonlocal boundary value problem [1]

$$-\alpha\left(\int_0^1 u(t)dt\right)u''(x)+[u(x)]^{2n+1}=0,\quad x\in[0,1],\quad u(0)=a,\ u(1)=b,$$

where u is the sought solution and α is a positive continuous function, was studied by J. R. Cannon and D. J. Galiffa, who proposed a numerical method based on an interval–halving scheme. Starting from their results, we provide a more general convergence theorem and suggest a different iterative procedure to handle the nonlinearity of the discrete problem.

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A Practical Trust-Region SQP Algorithm For Equality- and Bound-Constrained Optimization without Derivatives

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Keywords. Derivative-free optimization; equality constraints; trust-region SQP method; active-set method.

Derivative-free optimization (DFO) has enjoyed renewed interest over the past years, mostly motivated by the ever growing need to solve optimization problems defined by functions whose values are computed by simulation. In the last few years, a number of derivative-free optimization methods have been developed and especially model-based trust-region methods have been shown to perform well.

Here, we present a new interpolation-based trust-region algorithm which can handle nonlinear and nonconvex optimization problems involving equality constraints and simple bounds on the variables. Our new algorithm is an extension of the algorithm BCDFO which handles bound constraints by an active-set method and has shown to be very competitive [1]. It relies also on the technique of self-correcting geometry proposed by Scheinberg and Toint [2]. The objective and constraint functions are approximated by polynomials of varying degree (linear or quadratic). The equality constraints are handled by a trust-region SQP approach, where each SQP step is decomposed into normal and tangential components [3]. Special care must be taken in case an iterate is infeasible with respect to the models of the derivative-free constraints. Globalization is handled by using an Augmented Lagrangian penalty function as the merit function.

We present numerical results on a test set of equality-constrained problems from the CUTEr problem collection and on a real-life application from engineering design in space craft development.

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Learning Motion Patterns of Robotic Arm

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Keywords. Robotic arm; motion patterns; inverse kinematic; trajectory planning; neural networks.

Robotic arm motion learning often consists of solving inverse kinematics problem (the coordinate transformation from the visual coordinates to the joint angles vector of the arm [1]), path finding through obstacles with or without trajectory optimization [2]. Feedback mechanism for online motion correction can also be incorporated. Models, that mimics nature, often have less accurate (but faster) inverse kinematics planning and heavily relies on feedback system and motion corrections [3]. This also enables robotic arm to grab moving targets.

In this work, different approach to robotic arms motion learning is suggested. When motion begins, each joint gains initial velocities, which are corrected in future time frames. Initial velocities are learned by feed forward neural network. This model allows to mimic different types of motions, that exists in nature [4], like reflexes, stereotypical and fully coordinated motions, by varying joints velocities and frequency of corrective actions.

Experiments were carried out in visual environment.

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Multi-Objective Optimization Aided Drawing of Special Graphs

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Keywords. Multi-objective optimization; business process diagram; aesthetic looking graph.

A problem of drawing special graphs is considered. This problem, related to the drawing of aesthetically looking business process diagrams (BPD), has emerged while developing a business process management methodology oriented to managers and consultants either designing a new small/medium enterprize (SME) or searching for the possibilities to improve an existing one. The aesthetical attractiveness of a BPD depends on several criteria. For example, the following criteria greatly influence aesthetical attractiveness of the considered graphs: the total length of connectors, the number of crossings, the compatibility of the process sub-flows with the generalized top-down and left-right direction. Since these criteria can be measured quantitatively it seems reasonable to reduce the problem of the BPD visualization to a problem of multi-objective optimization.

In the present paper the relative importance of the relevant criteria of aesthetic attractiveness is discussed. The data from available publications is compared with the results of a psychological experiment with participation of our students. The goal of the psychological experiment was to rank the considered criteria and to evaluate their relative importance quantitatively. The results of the psychological experiment have been processed by the algorithm called Analytical Hierarchy Process.

Several multi-objective optimization algorithms have been tested with respect to the applicability of the considered problem. The results of the mentioned above psychological experiments have been used for the scalarization of the original multi-objective optimization problem. Some metaheuristic algorithms have been used for the solution of the obtained single-objective problem. Alternatively multi-objective optimization algorithms have been used to construct the sets of Pareto-optimal solutions. The conclusions are drawn on rationality of the applicability of different algorithms in different situations of the BPD visualization.

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Quasi-Monte Carlo Method and New Classes of Uniformly Distributed Sequences

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Keywords. Quasi-Monte Carlo method; quasi random numbers; uniform distribution; low discrepancy.

In numerical analysis, quasi-Monte Carlo method is used to compute integrals in higher dimension by low discrepancy sequences. The original Monte Carlo integration is based on sequences of random (or better, pseudorandom) numbers.

Monte Carlo and quasi-Monte Carlo methods are stated in a similar way. The idea is to approximate the integral of a function f on the d-dimensional hyper-cube $[0,1[^d$ as the average of the function evaluated at a set of points $x_1, \dots x_n$:

$$\int_{[0,1[^d} f(x)\,dx \simeq \frac{1}{n}\sum_{i=1}^{n} f(x_i)\,.$$

Random sequences provide, with probability 1, an approximation of order $O(\frac{1}{\sqrt{n}})$, while low discrepancy sequences assure an approximation of order $O(\frac{(\log n)^{d-1}}{n})$.

For integration in high dimension the usual Halton and Sobol sequences show some drawbacks, therefore it is important to construct new low discrepancy sequences. This can be done generalizing a construction due to Kakutani [1]. Some of the more significant result are contained in [2-4].

This is a research program which is developed by a group of researchers of the University of Calabria and the Technical University of Graz.

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Positivity Conditions in the Interpolation Problem by Weighted Cubic Splines

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Keywords. Weighted cubic spline; positivity.

At present, spline methods have become the main tools for solving the majority of problems involving the approximation of functions. These, naturally, include interpolation problems. Cubic splines of class C^2 are the basic and most universal tool because of their good approximation properties combined with simple computer implementation. However, in general, an interpolating cubic spline does not inherit such geometric characteristics as the preservation of sign of any derivative of the original function. It is well known that even the approximation of arbitrarily smooth functionsmay be accompanied by undesirable oscillations if the input data is not sufficiently "dense".

Miroshnichenko [1] suggested to use weighted splines in the monotonicity interpolation problem, and he presented a method for automatic selection of the weights. In this talk we suggest using the approach of the papers [2, 3] and we are studying the application of weighted cubic splines in the positivity interpolation problem.

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Computing the Fundamental Solutions for Equations of Electrodynamics and Elastodynamics

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Keywords. Maxwell's equations; elastodynamics; computation.

In the first part of this paper the time-dependent wave propagation in magnetoelectric (ME) (or bi-anisotropic) materials is considered. The electromagnetic wave propagation in ME materials is governed by Maxwell's equations with the special constitutive relations. In the present paper Maxwell's equations for these materials are written in the form of a symmetric hyperbolic system. A computer method for the computation of the fundamental solution of the time-dependent Maxwell's equations as well as the electric and magnetic fields from polarized pulse dipoles in homogeneous ME materials is suggested and implemented.

The time-dependent differential equations of elasticity for 3D quasicrystals (QCs) are considered in the second part of our paper. These elastic equations of 3D elasticity in QCs are more complicated than those of classical elasticity because in QCs a phason displacement field exits in addition to a phonon displacement. These equations of 3D elasticity in QCs are written in the form of a vector partial differential equation of the second order with symmetric matrix coefficients. A method of the numerical computation of the fundamental solution of this vector differential equation is proposed. This method is based on the Fourier transformation and some matrix computations. Computational experiments confirm the robustness of our method for the computation of the time-dependent fundamental solution of three-dimensional elastodynamics in QCs. This paper continues the research of works [1–3].

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Criteria of Ergodicity for p-Adic Dynamical Systems

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Keywords. Ergodicity; van der Put; coordinate functions.

Recently p-adic numbers found numerous applications in physics, cognitive science, genetics, see [1]. In particular, p-adic dynamical systems found applications in cryptography, see, for example, [2]. The problem of ergodicity for p-adic dynamical systems has a natural crytographic interpretation and therefore this problem is the topic of intensive study.

In general, to get the answer to the question whether the concrete p-adic dynamical system is ergodic or not one has to check its transitivity modulo p^n for every n. The main problem is to find algorithms which give the answer to the question about ergodicity without to appeal to infinite modulo p^n checking (which is useless for concrete numerical applications).

We restrict our study to the class of so called 1-Lipschitz functions, see the monograph [2], and present a number of easily checkable conditions of ergodicity. The basic technical tools are van der Put series, [3, 4] and usage of algebraic structure (permutations) induced by coordinate functions, [2], with partially frozen variables. Moreover, by using these representations we can consider non-smooth p-adic transformations.

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Reversible Semantics of Firewall's Operations

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Keywords. Reversible computations; dynamic cloud infrastructure; information security.

One of the actual challenges in computer science is to improve an information security of the high-performance cloud computing system. The semantic reversibility of firewall rules offers new opportunities for a parametric and structure adaptation of security appliances in the cloud environment. Such capabilities are especially important in the distributed systems when the parameters and characteristics of the computational services can change dynamically.

In the report the firewall rules are represented as the specific algebraic system. The operations of this algebra allow to perform formal transformations of active firewall rules for the current cloud configuration. During such transformation it is important to keep an integrity of the selected access control policy. It requires a consideration of the transformation from algebraic and semantic points of view. We propose an approach to improve the firewall's security service robustness that is called the semantic reversibility of filtering rules. The new formalism is based on the theory of categories and can be applied not only to the access control, but also to the intrusion detection or an intellectual prevention of the distributed systems.

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Optimization Methods for Real-Time Image Deconvolution on GPU Architectures

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Keywords. Image deconvolution; gradient projection methods; GPU.

Deconvolution techniques are required in many imaging applications for mitigating the distortions produced by the acquisition system. Thus, high-performance deconvolution algorithms become crucial to avoid strong delay in the data analysis pipeline, especially in case of large-scale imaging problems, such as those arising in astronomy and microscopy. In this work we present effective deconvolution approaches obtained by following two main directions: using accelerated deconvolution algorithms and exploiting Graphics Processing Units (GPUs). An accelerated deconvolution algorithm is derived from a scaled gradient projection (SGP) method [2] for the solution of the constrained optimization problems provided by the maximum likelihood approach and, for the regularized version, by the maximum a posteriori approach. The SGP method is an iterative first-order scheme that, due to its simplicity, is well suited to be implemented on GPU devices. In this work we discuss an extended SGP version that combines the acceleration property with the ability to face 3D problems and to integrate a boundary-effect correction according to the approach proposed in [1]. Numerical experiments on large-scale 2D and 3D microscopy data show that the proposed approaches provide a robust tool for real-time deconvolution, when implemented on modern GPU architectures.

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Global Optimization Issues in Problems of Matrix Low Rank Approximation

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Keywords. Global optimization; low-rank approximation; Hankel matrix; singular value decomposition.

In this talk we illustrate some optimization challenges arising in the following two problems of matrix low rank approximation: (a) structured low rank approximation (SLRA) problem, and (b) weighted low rank approximation (WLRA). Both problems have wide range of applications and for both problems the global optimization issues are not yet resolved and not even understood.

SLRA can be described as the problem of finding a low rank approximation of an observed matrix which has the same structure as this matrix (such as Hankel). We demonstrate that the optimization problem arising is typically very difficult: in particular, the objective function is multiextremal even in very simple cases. We believe that the difficulties described in approximating a solution of the SLRA problem open huge possibilities for the application of both stochastic and Lipschitz-based methods of global optimization.

A traditional method of approximating the solution of the Hankel SLRA problem is based on the use of Alternating Projections (AP) between the space of low rank matrices (obtained via the singular value decomposition) and the space of Hankel matrices (by averaging over the anti-diagonals). Despite AP iterations are known to behave poorly it is the main method used in practice. Other methods known to matrix algebra and signal processing communities are also local and do not guarantee the convergence to the global minimizer of the objective function. We extend AP by introducing backtracking and stochasticity into the projections. Following the results of [1] we show that the corresponding algorithms guarantee the global convergence and indeed show very promising results in practical applications.

Global optimization problems of different sort arise in WLRA problems. These problems are mostly related to the over-parametrization of the solutions and therefore to the presence of huge valleys and ridges in the objective functions. As a result, AP algorithms get stuck on their to the optimal solution. Once again, some stochasticity helps to improve the behaviour of algorithms.

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On Discrete Representation of Pareto Set in Non-Convex Multi-Objective Optimization

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Keywords. Multi-objective optimization; global optimization; branch-and-bound.

Multi-objective optimization is a research area rich with various approaches [1,2]. However, a general aspect of many of approaches is the construction of a discrete representation of the set of Pareto-optimal solutions. The requirements to such a representation in various algorithms can be rather different. For example, it can be sufficient to find a rough approximation of the Pareto-optimal set to aid the selection of a starting point for interactive search. Alternatively, a possibly complete representation can be needed. In the present paper several algorithms for non-convex continuous and combinatorial multi-objective optimization problems are considered.

Two approaches are considered to the optimal construction of discrete representation of Pareto sets of continuous non-convex problems. First: an algorithm optimal with respect to a statistical model is developed; this algorithm is a generalization of the single-objective P-algorithm (see, [3]) to the case of multi-objective optimization. The second algorithm is the one step worst case optimal algorithm with respect to the class of Lipschitz functions.

For combinatorial multi-objective optimization we consider multi-objective branch-and-bound which is able to find the exact Pareto-optimal set and metaheuristics for approximation of the Pareto-optimal front. We discuss some problems of combinatorial multi-objective optimization like cell formation, aesthetic visualization of business process diagrams, and competitive facility location.

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A New Space Discretization of the 1D Quasi-Gas Dynamic System of Equations and the Entropy Balance Equation

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Keywords. Gas dynamics; finite-difference schemes; the entropy balance equation.

In gas dynamics, the law of non-decreasing total entropy plays the key role. The law holds for the quasi-gas dynamic (QGD) system of equations [1,2]. The corresponding kinetic finite-difference schemes work well in many test and practical gasdynamic computations. However, for the standard space discretization of the QGD system, the validity of this law cannot be guaranteed even in the spatially 1D case due to appearance of mesh imbalance terms.

We construct a new conservative three-point and symmetric in space discretization of the QGD system such that the entropy balance equation of the proper form holds and the non-negativity of the entropy production is valid [3,4]. This takes place in the presence of the mass force and a heat source. Essential elements of the new method are several non-standard space averages including nonlinear "logarithmic" ones for the density and the internal energy.

The accomplished numerical experiments also give promising results.

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