BOOK OF ABSTRACTS

The 3rd International Conference and Summer School

Numerical Computations: Theory and Algorithms NUMTA 2019

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edited by

Yaroslav D. Sergeyev
Dmitri E. Kvasov
Marat S. Mukhametzhanov
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University of Calabria, Rende (CS), Italy
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Book of Abstracts of the 3rd International Conference and Summer School

Numerical Computations: Theory and Algorithms

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Le Castella - Isola Capo Rizzuto
Crotone, Italy
June 15-21, 2019

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NUMERICAL COMPUTATIONS: THEORY AND ALGORITHMS
Third International Conference and Summer School NUMTA-2019
15-21 June 2019, Le Castella - Isola Capo Rizzuto (Crotone), Italy

Dear Participants,

Welcome to the Third Triennial International Conference and Summer School NUMTA-2019 "Numerical Computations: Theory and Algorithms". The Conference is organized by the University of Calabria, Department of Computer Engineering, Modeling, Electronics and Systems Science, Italy. We are proud to inform you that, as the previous two editions, NUMTA-2019 is organized in cooperation with the Society for Industrial and Applied Mathematics (SIAM), USA. This edition has been organized under the high patronage of the municipality of Crotone - the city of Pythagoras and his followers, the Pythagoreans. In fact, Pythagoras has established the first Pythagorean community in this city in the 6th century B.C. It is a very special feeling to return to these holy for any mathematician places with a conference dedicated to numerical mathematics.

This edition of the NUMTA Conference is dedicated to the 80th birthday of Professor Roman Strongin. For the past 50 years Roman Strongin has been a leader and an innovator in Global Optimization being an important field of Numerical Analysis having numerous real-life applications. His book on global optimization published in 1978 was one of the first in the world on this subject. Now it is a classic and has been used by many as their first introduction and continued inspiration for global optimization. Since that time Roman has published numerous books and more than 400 papers in several scientific fields and has been rewarded with many national and international honors including the President of the Russian Federation Prize. For decades Roman served as Dean, First Vice-Rector, and Rector of the famous Lobachevsky State University of Nizhniy Novgorod. Since 2008 he is President of this university. He is also Chairman of the Council of Presidents of Russian Universities, Vice-President of the Union of the Rectors of Russian Universities, and Chairman of the Public Chamber of the Nizhniy Novgorod Region.

The goal of all NUMTA Conferences is to create a multidisciplinary round table for an open discussion on numerical modeling nature by using traditional and emerging computational paradigms. The NUMTA-2019 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, machine learning, 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 30 countries participate at the Conference: Argentina, Bulgaria, Canada, China, Czech Republic, Estonia, Finland, France, Germany, Greece, India, Iran, Italy, Japan, Kazakhstan, Latvia, Lithuania, Netherlands, Philippines, Portugal, Romania, Russia, Saudi Arabia, South Korea, Spain, Switzerland, Thailand, Ukraine, UK, and USA.

Authors of selected talks will be invited to submit full papers to special issues of the international journals Applied Mathematics and Computation and Journal of Computational and Applied Mathematics (both produced by Elsevier) and Soft Computing (produced by Springer) dedicated to the Conference.

The Organizing Committee expresses its gratitude to institutions that have offered their support to the international conference NUMTA-2019. This support was essential for the success of this event:

- University of Calabria (Italy);
- 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);
- Springer;
- International Association for Mathematics and Computers in Simulation;
- International Society of Global Optimization.

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 fields.

Yaroslav D. Sergeyev
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Plenary lectures

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Infinite Games on Finite Graphs using Grossone

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Keywords. Infinite games; Grossone; Finite Automata.

Finite board games that are played to infinity may sound like computer science fiction. Indeed, following the traditional Turing machine model, a computation is complete when it halts and produces some type of result. However when a game is played to infinity, it is implied that the game continues for an indefinite period (play continues without bound). It is easily seen that in a multiprogramming computer, when one process is satisfied, the operating system must continue and select another process to be executed. This is the ongoing operation and hence computation actually becomes a continuation action and, theoretically, without end. In the seminal work by Robert McNaughton (see [1]) a model of infinite games played on finite graphs is developed. The model proposes two players, Red and Black, that take turns moving from vertex to vertex along the directed edges of a bipartite graph, where each move corresponds to a different game configuration. This paper presents a new model of infinite games played on finite graphs using the Grossone paradigm (see [2] and [3]). The new Grossone model provides certain advantages such as allowing for a draw, which can result and are not uncommon in board games, and a more clear and decisive (accurate) method for determining the winner. Then, and subsequently, motivated by this infinite duration game model, a model to represent communication networks problems is proposed. Such a game model will be called an update network.

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Recent advances on the use of ① in optimization and regularization problems

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Keywords. Optimization problems, regularization problems, ①, l_0 minimization.

In recent years, several classical optimization problems have been tackled using the novel approach to infinite and infinitesimal numbers proposed by Sergeyev [1–3]. The use of ① has been beneficial both in defining new approaches in constrained optimization [4] (for example, new differentiable exact penalty methods) and unconstrained problems (for example, conjugate gradient methods for indefinite matrices, variable metric approach to nonsmooth optimization).

After a review of the most important results in this context the talk will concentrate on regularization problems with smoothed l_0 penalty. In order to avoid the difficulties due to the use of the l_0 norm, two different approaches have been proposed in literature. The first is to replace the l_0 norm with the l_1 or l_2 norm; the second technique uses a smooth function that will approximate the l_0 norm of a vector. This approach requires the usage of a parameter δ that must converge to 0. This difficulty can be avoided by using the novel approach to infinite and infinitesimal numbers. The methods used can be extended to classification and regression problems.

Acknowledgements.
This research was supported by the grant from Indam-GNCS; 2018.

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Karush-Kuhn-Tucker Proximity Measure for Convergence of Real-parameter Single and Multi-Objective Optimization

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Keywords. KKT optimality conditions; proximity measure; convergence, multi-objective optimization.

The proximity of an obtained solution to theoretical optimum is always the first priority to any optimization algorithm developer. In constraint optimization problems, Karush-Kuhn-Tucker (KKT) optimality conditions can at most determine a binary decision about a solution - a likely candidate of being the optimum, or not an optimum. However, further information about a solution's proximity to the theoretical optimum either in the variable space or in the objective space would be valuable to the algorithm developer. Such information will also be valuable to the applicationists in assessing the solution's quality and acceptability as a final solution. In this talk, we shall present a KKT proximity measure (KKTPM) based on approximate KKT point concepts suggested in the literature. KKTPM exhibits a high correlation of the difference from optimal objective value to the KKTPM value., thereby making KKTPM a measure of convergence to the true optimum. The concept of KKTPM is also extended for multi-objective optimization to determine the proximity of a solution's objective vector from the theoretical efficient set, without any knowledge of the theoretical efficient set. Results on standard two to 15-objective test problems and on a few engineering design optimization problems will be shown. The computational burden of optimization-based KKTPM calculation is reduced using a direct approach in which an approximate KKTPM is computed. KKTPM has also been used to improve the performance of an evolutionary multi-objective optimization (EMO) algorithm in a unique way. Some other extensions and applications of the KKTPM will also be discussed to highlight the usefulness of the proposed KKTPM in single and multi-objective optimization. For further information, refer the following articles:

References

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Numerical modeling of flow in fractured porous media and fault reactivation

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Keywords. Fractured porous media; Frictional contact.

The study of flow in heterogeneous and fractured porous media finds application in several fields, from material science to bio-medicine, and geophysics. In the last here we have investigated several numerical techniques to describe flow in porous media in the presence of fracture networks, mainly with applications in subsurface flows.

Fractures in the subsurface are present with a very large variation of spatial scales, they may form complex networks and influence the underground flow considerably.

A common characteristic of fractures is the fact that their width (technically called aperture) is much smaller than the other dimensions. Therefore, it may be convenient to model them as as one-codimensional manifolds immersed in the porous matrix rock, possibly forming a network. We have then a coupled differential problem formed by the equations for the flow in the rock matrix and a reduced model posed on the tangential plane of the fracture. The model is completed by suitable coupling conditions describing the mass flow interchange between fracture and rock matrix and, in the case of networks, coupling conditions at the fracture intersections. We will review some recent results concerning the properties of numerical schemes for this class of problems.

In the case of faults, alteration of the flow field due, for instance, human activity, may alter the stress distribution and cause the risk of (micro)seismic activity (fault activation). In this situation the flow problem has to be coupled with a mechanical model of the rock, giving rise to a Biot model, and a frictional model to account the possibility of fault slip. We will present recent studies of a technique based on the minimization of a non-linear functional that allows to impose the friction condition without resorting to Lagrange multipliers.

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Precision Algorithms

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Keywords. Nonlinear algorithms, neural networks conservation laws

Many algorithms contain parameters or specific nonlinear steps that require problem specific tuning for the algorithm to perform optimally. Classic examples include the definition of shape parameter in radial basis interpolation or the detection of bad cells when one solves conservation laws with high-order methods. However, choosing such parameters or local strategies is often complicated and difficult to achieve in an optimal manner since they depend on the solution/iteration etc. Another common bottleneck is a specific element of a algorithm in which the majority of the computational effort is spent, e.g., multi-scale problems in which the microscopic solver is very expensive.

In this talk we shall discuss the potential of using artificial neural networks to overcome such bottlenecks to allow optimal local parameter choices and a resulting acceleration or improved performance of the algorithm.

After a brief introduction to neural networks, we demonstrate this general idea through a number of specific examples, primarily motivated by challenges associated with the numerical solution of conservation laws.

While exemplified trough specific examples, the overall philosophy is general and conclude with a slightly more general discussion of the potential of such enhanced methods, referred to in this talk as precision algorithms.

Numerical differentiation on the Infinity Computer and applications for solving ODEs and approximating functions

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Keywords. Ordinary Differential Equations, BS-Hermite-Obrechkov spline approximation, Initial Value Problems, grossone (①), Infinity Computer.

The computation of derivatives using the Infinity Computer arithmetic has recently motivated the analysis of algorithms for the numerical solution of ordinary differential equations that involve higher derivatives. Moreover the relation of some of these algorithms with spline quasi-interpolation methods of differential type allowed us to use the infinite computer arithmetic also in the context of approximation theory.

After a review of the most important results already reached in this context, the talk will deal with Hermite-Obrechkov methods for the solution of ODEs and their related spline quasi-interpolation schemes. We shall see that the use of ① produces a precise value of the total derivative without explicitly evaluating its analytical expression in terms of the derivatives of f. The final goal of this new approach is to improve the computational effort associated with the evaluation of the involved derivatives and make them competitive with respect to more standard integrators. A novel application that will be described is the use of the Infinity Computer also in the approximation context, using ① to compute the input data of quasi-interpolation schemes.

Acknowledgements. This work was funded by the INdAM-GNCS 2018 Research Project "Numerical methods in optimization and ODEs" (the author is member of the INdAM Research group GNCS).

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Generalizations of the intermediate value theorem for approximations of fixed points and zeroes of continuous functions

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Keywords. Bolzano theorem; Bolzano-Poincaré-Miranda theorem; intermediate value theorems; existence theorems; fixed points; nonlinear equations; numerical optimization.

Generalizations of the tractional intermediate value theorem are presented. The obtained generalized theorems are particular useful for the existence of solutions of systems of nonlinear equations in several variables as well as for the existence of fixed points of functions and the localization and computation of extrema of objective functions.

The only computable information required by the numerical methods based on these generalized theorems is the algebraic sign of the function that is the smallest amount of information (one bit of information) necessary for the purpose needed, and not any additional information. Thus, these numerical methods are of major importance for tackling problems with imprecise (not exactly known) information. This kind of problems occurs in various scientific fields including mathematics, economics, engineering, computer science, biomedical informatics, medicine and bioengineering among others. This is so, because, in a large variety of applications, precise function values are either impossible or time consuming and computationally expensive to obtain.

Furthermore, these methods are particularly useful for tackling various problems where the corresponding functions take *very large* and/or *very small* values.

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Uniformly distributed sequences and space-filling

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Keywords. Computer experiments; space covering; global optimization; kernel methods; discrepancy; dispersion

Let X be a compact subset of R^d and f be a black-box function on X. A standard objective in global optimization, computer experiments as well as in diverse applications is to approximate the behaviour of f on X from only a few evaluations in X. When little is known about the function, space-filling design is advisable: typically, points of evaluation spread out across the available space are obtained by minimizing a certain criterion measuring distance to uniformity.

In this talk, we follow [1,2] and review several classes of uniformity criteria including dispersion (or covering radius) and various discrepancies and establish connections between some of these criteria. We also investigates connections between design for integration (quadrature design), construction of the (continuous) best linear unbiased estimators for the location model, and minimization of energy (kernel discrepancy) for signed measures. Integrally strictly positive definite kernels define strictly convex energy functionals, with an equivalence between the notions of potential and directional derivative, showing the strong relation between discrepancy minimization and more traditional design of optimal experiments. In particular, kernel herding algorithms, which are special instances of vertex-direction methods used in optimal design, can be applied to the construction of point sequences with suitable space-filling properties.

We will pay special attention to kernels with singularities where the space-filling sequences have some very attractive properties of but the machinery of the reproducing kernel Hilbert spaces is not applicable. Various regularization techniques should be used in practise for solving arising optimization problems. In doing this we have to work with infinitesimals; in doing so we would advocate the use of the infinity computer of Ya.Sergeyev [3]. We will also observe big differences between the cases when the dimension d is small and when d is large.

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Tutorials

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Vector kinetic approximations to fluid-dynamics equations

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Keywords. Kinetic numerical schemes, Naviers-Stokes Equations, Hyperbolic problems

A singular semilinear hyperbolic approximation to the Euler and the incompressible Navier-Stokes equations in 2D, inspired by the kinetic theory, is considered. This approximation is interesting for numerical reasons, but also as a fully hyperbolic approximation.

In the first part of the talk, I will illustrate the structure of this approximation and its numerical advantages, already presented in [3]. Then, I will present a result of convergence of the vector-BGK to the incompressible Navier-Stokes equations in the diffusive scaling, see [1, 2].

This result deeply relies on the dissipative properties of the system and on the use of an energy which is provided by a symmetrizer whose entries are weighted in a suitable way with respect to the diffusive parameter. This convergence is valid for smooth solutions and it is global in time.

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Grossone-based Infinity Computing with Numerical Infinities and Infinitesimals

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Keywords. Infinity Computing; Grossone; Numerical Computation

In this tutorial, a recently developed computational methodology is described (see patents [1] and a comprehensive description given in [2]). It allows one to execute *numerical* (not symbolic) computations with a variety of infinities and infinitesimals based on the principle *'The part is less than the whole'* applied to all quantities: finite, infinite, and infinitesimal. This methodology does not contradict Cantor, Levi-Civita, and Robinson evolving their ideas in a more applied way and moving from purely symbolic to numerical calculus. A computational device called the *Infinity Computer* (see patents [1]) is used to work numerically with infinite and infinitesimal numbers that can be written in a positional system with an infinite base that is denoted by the symbol ① called *Grossone*. A number written in this numeral system can have several infinite and infinitesimal parts, a finite part can be either present or absent. On a series of theoretical and practical examples dealing with Turing machines, set theory, numerical differentiation, optimization, divergent series, ODEs, fractals, etc. (see, e.g., [1,3,4]) it is shown that the new way of counting can be very useful. Obtained results and their accuracy are repeatedly compared with answers provided by traditional tools used by mathematicians to work with objects involving infinity.

The *Infinity Calculator* working with the introduced infinities and infinitesimals numerically is shown during the presentation. A lot of information can be found at the dedicated web page `http://www.theinfinitycomputer.com`

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Design optimization techniques for industrial applications: challenges and progress

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Keywords. Design optimization; metamodel; trust region strategy.

Current industrial applications of design optimization exhibit several features that are not yet adequately addressed by commercially available optimization tools:

- Large scale (1000+ design variables) optimization problems with expensive (10+ hours) response function evaluations that are polluted by numerical noise
- Discrete optimization with even moderately expensive response functions
- Multidisciplinary optimization in an industrial setting
- Optimization with non-deterministic responses.

The presentation discusses recent progress towards addressing these issues by identifying general trends and appropriate methods for solving large scale optimization problems focusing on the trust region-based metamodelling techniques [1], specifically addressing the issues of numerical noise and uncertainty and occasional failures of the solvers to produce responses [2,3]. The use of variable fidelity responses is identified as a highly beneficial approach as it allows to establish high accuracy metamodels using only small-scale sampling of the high fidelity responses. The presentation is illustrated by examples of industrial optimization problems with a focus on the aerospace sector [4].

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Special sessions

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Approximation: methods, algorithms and applications

Organizers:
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Laplace Transform Inversion for multiexponential decay data by smoothing L-splines

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Keywords. L-spines; Laplace transform; Bernstein bases; B-spline bases.

In many applications, the definition of fitting models that mimic behaviors of experimental data to numerically investigate problems is a challenging issue. In this paper a data-driven approach to represent (multi)exponential decay data is presented. More in details, a functional description of these information give the possibility to adopt powerful mathematical tools for data analysis such as the Laplace transform [1]. We propose a fitting model that is a piecewise smoothing L-spline satisfying a suitable differential operator tailored to represent the data behaviour. The main contribution is to define B-spline like functions locally represented by Bernstein-like bases satisfying Hermite interpolation conditions ([2], [3], [4]). Numerical experiments on the inversion of real multi-exponential decay data of a Laplace Transform have been carried out in a case study.

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An Adaptive Refinement Scheme for Radial Basis Function Collocation

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Keywords. Meshless methods; Adaptive algorithms; Elliptic PDEs.

The problem of constructing adaptive meshless-based collocation methods is widely studied in literature, see e.g. [1,2,3,4] and references therein.

In this paper we present an adaptive refinement algorithm for solving elliptic partial differential equations via a radial basis function (RBF) collocation method. The adaptive scheme is based on the use of an error indicator, which is characterized by the comparison of two RBF collocation solutions evaluated on a coarser set and a finer one. This estimate allows us to detect the areas that need to be refined by adding collocation points. Numerical results support our study and points out the effectiveness of our algorithm.

Acknowledgements.

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Interpolation by bivariate quadratic polynomials and applications to the scattered data interpolation problem

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Keywords. Multinode Shepard methods; Rate of convergence; Approximation order.

As specified by Little [2], the triangular Shepard method can be generalized to higher dimensions and to set of more than three points. In this line, the hexagonal Shepard method has been recently introduced by combining six-points basis functions with quadratic Lagrange polynomials interpolating on these points and the error of approximation has been carried out by adapting to the case of six points the technique developed in [1]. As for the triangular Shepard method, the use of appropriate set of six-points is crucial both for the accuracy and the computational cost of the hexagonal Shepard method. In this talk we discuss about some algorithms to find useful six-tuple of points in a fast manner without the use of any triangulation of the nodes.

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A 3D efficient procedure for Shepard interpolants on tetrahedra

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Keywords. Scattered data interpolation; Fast algorithms; Approximation algorithms.

The need of scattered data interpolation methods in the multivariate framework and, in particular, in the trivariate case, motivates the generalization of the fast algorithm for triangular Shepard method [4, 3] presented in [2]. There a block-based partitioning structure procedure introduced in [1] was applied to make the method very fast in the bivariate setting. Here the searching algorithm is extended, it allows to partitioning the domain and nodes in cubic blocks and to find the nearest neighbor points that need to be used in the tetrahedral Shepard interpolation.

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Comparison of Shepard's like methods with different basis functions

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Keywords. Shepard method; Quasi-interpolation operators; Fast approximation methods.

The problem of reconstruction of an unknown function from a finite number of given scattered data (x_i, f_i), that is data which consist of functional values corresponding to points which do not obey any structure or order between their relative locations, is well known and well studied in approximation theory. Several methods both which require a mesh (here we mention that one based on multivariate splines, finite elements, box splines) or meshless methods, mainly based on radial basis functions, have been developed with this goal and are successfully applied in different contexts. Recently [2], it has been pointed out the need of fast approximation methods which overcome the high computational cost and the slowness of interpolation schemes which entail the solution of large linear systems or the use of elaborated mathematical procedures to find the values of parameters needed for setting those schemes. The Shepard method [3] and some of its variations [1] belong to this class of methods. In this talk we compare methods which are variations of the classic Shepard method obtained by considering different basis functions.

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A SVE approach for the numerical solution of ordinary differential equations

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Keywords. Approximation; Ordinary Differential Equation; Numerical Differentiation; Singular Value Expansion; Volterra Integral Equation.

The derivative operator can be easily reformulated as a Volterra integral operator of the first kind, see [1] for a detailed discussion. So the singular value expansion (SVE) of the kernel of such integral operator [2] can be used to obtain new numerical methods to solve ordinary differential equations (ODE).

We present an iterative scheme where global error in the solution of the ODE is gradually reduced at each step. The global error is approximated by using the system of the singular functions in the aforementioned SVE.

Some experiments are used to show the performances of this proposed numerical method.

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Edge-driven interpolation with discontinuous kernels and applications in medical imaging

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Keywords. Scattered Data Interpolation of Discontinuous functions, Edge-driven Interpolation, Interpolation Artifacts, Variably Scaled Discontinuous Kernels, Classification of Images with Kernel Machines.

To construct an interpolation scheme that maintains the edges of a function we study an edge-driven interpolation method based on variably scaled discontinuous kernels [1]. As a main result obtained in [2], we present a characterization for the native space generated by these discontinuous kernels and provide, similar as in [3], Sobolev type error estimates for the interpolation error. Our numerical experiments confirm that the theoretical convergence rates given in terms of a local fill distance are correct. We further study the effect of perturbations of the scaling function on the resulting interpolant and demonstrate that an accurate estimate of the discontinuities is necessary in order to obtain a faithful interpolation.

If this information of the discontinuities is not a priori given, we need an edge detector to estimate the discontinuities. For this purpose, we use kernel machines that are trained with the given scattered data. The results of our interpolation method applied to a problem in medical imaging are promising and show that reconstruction artifacts, as for instance ringing and truncation artifacts, can be sensibly reduced in the interpolation process.

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A New Remez-type Algorithm for Best Polynomial Approximation

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Keywords. best polynomial approximation; Remez algorithm; interpolation.

The best approximation problem is a classical topic of the approximation theory and the Remez algorithm is one of the most famous methods for computing minimax polynomial approximations [2].

We present a slight modification of the Remez algorithm where a new approach to update the trial reference is considered. In particular at each step, given the local extrema of the error function of the trial polynomial, the proposed algorithm replaces all the points of the trial reference considering some ad hoc oscillating local extrema and the global extremum of the error function. Moreover at each step the new trial reference is chosen trying to preserve a sort of equidistribution of the nodes at the ends of the approximation interval. This method is particularly appropriate when the number of the local extrema of the error function is very large.

Several numerical experiments are performed to assess the real performance of the proposed method in the approximation of continuous and Lipschitz continuous functions. In particular, we compare the convergence properties of best approximants computed with different numerical methods. Among the other we consider the algorithm proposed in [3] where an update of the Remez ideas for best polynomial approximation in the context of the chebfun software system is studied (see [1]).

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Gauss and anti-Gauss quadrature rules applied to integral equations of the second kind

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Keywords. Gauss quadrature; anti-Gauss quadrature; integral equations.

At the beginning of the nineteenth century Carl Friedrich Gauss developed an interpolatory formula having the maximal algebraic degree of exactness. Today such a rule is known as the Gauss quadrature formula [1].

In 1996 Dirk Laurie was the first to coin the anti-Gauss quadrature rule, an interpolatory formula designed to have the same degree of exactness of the Gauss formula and an error precisely opposite to the error of the Gauss rule, if applied to polynomials having a specific degree [2].

The aim of this talk is to present a global approximation method based on the above quadrature rules for the following integral equation of the second kind

$$f(y) - \int_{-1}^{1} k(x,y)f(x)w(x)dx = g(y), \quad y \in [-1, 1]$$

where f is the unknown function, k and g are two given functions and $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$ is a Jacobi weight with parameters $\alpha, \beta > -1$.

The convergence and the stability of the proposed method will be discussed in suitable weighted spaces and numerical tests will show the accuracy of the approach.

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Advanced numerical treatment of an accurate SPH method

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Keywords. IFGT; SPH; GPUs.

The summation of Gaussian kernel functions is an expensive operation frequently encountered in scientific simulation algorithms and several methods have been already proposed to reduce its computational cost. In this work, the Improved Fast Gauss Transform (IFGT) [1] is properly applied to the Smoothed Particle Hydrodynamics (SPH) method [2] in order to speed up its efficiency. A modified version of the SPH method is considered in order to overcome the loss of accuracy of the standard formulation [3]. A suitable use of the IFGT allows us to reduce the computational effort while tuning the desired accuracy into the SPH framework. This technique, coupled with an algorithmic design for exploiting the performance of Graphics Processing Units (GPUs), makes the procedure promising as shown by preliminary numerical simulations.

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On non-parametric regressions by means of multivariate polysplines

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Keywords. Non-parametric regression; polysplines; smoothing polysplines.

One of the main approaches of the modern Data Analysis and Machine Learning is to use regressions for data interpolation/extrapolation. In the case of one-dimensional data there is a large variety of methods many of which are using non-parametric regressions based on splines, or alternatively spline regressions. The splines used are the usual polynomial, trigonometric, or generalized splines, as the so-called L-splines and Chebyshev splines. We have to mention the names of the pioneers and most active researchers in the area, as G. Wahba, L. Schumaker, T. Lyche, J. Ramsay, Ch. Gu and others. From the point of view of Data Analysis, it is important that for these regressions, the spline approach provides estimates for error, Cross-validation, Confidence intervals, and Residuals. We refer to the monographs [4], [2] and the references therein. On the other hand for the case of multivariate data the usual approaches use Kriging, Thin Plate Splines, Radial Basis Functions, for which there is still a limited success in obtaining regressions with fast computational methods, as well as fast computation of estimates for the error, the Cross-validation scores, Confidence intervals, and the Residuals. We have recently proposed in [3] to use multivariate polysplines developed in [1] for construction of non-parametric regressions, and regression polysplines. For these new methods it is possible to find fast methods for their computation as well as efficient computation of the error, Cross-validation scores, Confidence itnervals, and Residuals.

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Weighted polynomial approximation on the square by de la Vallée Poussin means

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Keywords. Approximation by Polynomials; Polynomial Interpolation; de la Vallée Poussin means; Orthogonal Polynomials

The talk deals with the generalization of discrete de la Vallée Poussin means on the square, obtained via tensor product by the univariate case [1]. Pros and cons of such a kind of filtered approximation are discussed. In particular, under simple assumptions on the involved Jacobi weights, we get near–best discrete approximation polynomials in the space of all locally continuous functions on the square with possible algebraic singularities on the boundary, equipped with the weighted uniform norm. In the four Chebychev cases, these polynomials also interpolate the function. Moreover, for almost everywhere smooth functions, the Gibbs phenomenon appears reduced. Comparison with other interpolating polynomials are proposed [2], [3].

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Recovering discontinuous functions via local multiquadric interpolation with adaptive nonlinear estimate of the shape parameter

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Keywords. Radial basis functions; Jump discontinuity; Weighted Essentially Non-Oscillatory methods; Adaptive parameter; Approximation order.

We discuss a new approach for the reconstruction of discontinuous one dimensional functions. It consists in applying a parameter-dependent local multiquadric interpolant that incorporates the ENO/WENO (Essentially Non Oscillatory/ Weighted ENO) techniques in the computation of the locally optimized shape parameter. The resulting nonlinear adaptive estimation of the shape parameter leads to accurate reconstructions in the smooth regions and to sharp solution profiles near jump discontinuities avoiding Gibbs phenomena. Differently from what proposed in [1], [2] this is a true radial WENO method that does not revert to classical polynomial WENO approximation near discontinuities. We present also some numerical examples that confirm the theoretical approximation orders.

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On some applications of generalized Kantorovich sampling operators

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Keywords. Sampling theory; Kantorovich sampling operators; approximation.

In this talk we consider a construction of fractional derivative masks for image edge detection and enhancement, based on generalized Kantorovich sampling operators. Edge detection and image enhancement methods, based on derivatives are well-known. Recently there is development to use several generalized fractional derivatives instead of the classical derivetaives of order 1 and 2 (see [2] and references cited there). For practical application of derivatives to images we need masks. For the classical case the Sobel masks are well-known. We introduce a construction of fractional derivative masks based on generalized sampling operators. For $f \in C(\mathbf{R})$ the generalized sampling operators are given by ($t \in \mathbf{R}$; $W > 0$;)

$$(S_W f)(t) := \sum_{k=-\infty}^{\infty} f(\frac{k}{W})s(Wt-k), \quad s \in L^1(\mathbf{R}), \quad \sum_{k\in\mathbf{Z}} s(u-k) = 1. \tag{1}$$

Generalized sampling operators (1) are a natural way to represent images. Such representation gives us a possibility to define different derivative masks, also for fractional derivatives. We use generalized Kantorovich sampling operators, introduced in [1], for more flexibility of the construction of masks.

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Numbers, Algorithms and Applications (Pythagorean Stream)

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New approaches to basic calculus: an experimentation via numerical computation

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Keywords. Numerical computing; mathematics education; grossone.

The introduction of the first elements of calculus both in the first university year and in the last class of high schools, presents many problems both in Italy and abroad. Emblematic are the (numerous) cases in which students decide to change their course of study or give it up completely cause the difficulties with the first exam of mathematics, which usually deals with basic calculus.

The central part of the talk concerns an educational experimentation involving above all some 5th classes of the IPS "F. Besta" in Treviso (IT), with partecipants' age about 19 years old, and also other classes. The project aims to explore the teaching potential offered by non-classical approaches to calculus jointly with the so-called "unimaginable numbers". In particular, we employed the computational method proposed by Y.D. Sergeyev (see, e.g., [3]) and widely used in mathematics, applied sciences and, recently, also for educational purposes.

In the talk there will be illustrated tools, investigation methodologies, collected data (before and after the teaching units), and the results of various class tests.

Lastly, we will also give some hints about recent related researches from analytic mechanics to supertrack functions and chaos theory, following the common thread of numerical computing and simulation.

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From the ancient Pythagorean School to contemporary mathematical models: paradoxes of the infinite and ontological dilemmas

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Keywords. Infinite; Greek Philosophy; grossone.

Since the birth of philosophy in ancient Greece, the concept of infinite has been closely linked with that of contradiction and, more precisely, with the intellectual effort to overcome contradictions present in an account of Totality as fully grounded. The present work illustrates the ontological and epistemological nature of the paradoxes of the infinite, focusing on the theoretical framework of Aristotle, Kant and Hegel. Interestingly, Aristotle solves the dilemmas of the infinite by hypothesizing a finite universe, by denying the existence of "actual" infinite and by supposing a non-dimensional entity which is at the origin of any movement and alteration of matter and which is beyond empirical verification: such a move cannot be embraced by modern philosophy and by modern mathematics, for different reasons. The work also attempts to realize an ontological interpretation of the necessity of mathematical instruments such as limits and infinitesimals and of their coexistence with paradoxes of the infinites and infinitesimals. Recent conceptual mathematical solutions to these paradoxes, such as Sergeyev's notion of grossone, are then compared with Hegel's notion of true infinite in their pragmatic significance.
The so-called "unimaginable numbers", also, can be considered as a subcase of the same Hegelian approach to the systematization of notions threatening the rationality and the compactness of experience.

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Numerical problems in XBRL reports and the use of blockchain as trust enabler

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Keywords. Financial models, blockchain, laws of Bradford and Zipf.

Financial statements are formal records of the financial activities that companies use to provide an accurate picture of their financial history. Their main purpose is to offer all the necessary data for an accurate assessment of the economical situation of a company and its ability to attract stakeholders. Our goal is to investigate how blockchain can be used for improving trustworthiness in the published financial reports. Our contribution is threefold: (i) providing a methodology to automatically evaluate and validate the consistency of the generated reports, (ii) to use Blockchain to store information as an immutable and uninterruptible worldwide database, (iii) to apply numerical tools to detect possible errors or even frauds in the reports.
For (i) we use ASP (answer set programming) to automize reasoning on the XBRL data. For (ii) we analyze the implementation of smart contracts on the Ethereum Blockchain. For (iii) we explore the so called Bradford's and Zipf's laws as tools for checking numerical values in the specific domain of company balance sheets.
For a possible use of an ASP language to analyse XBRL financial reports and a preliminary experimental data on some real world companies, see [1,3].

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Modelling on human intelligence a Machine Learning System

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Keywords. Emotion Recognition; Machine Learning; Data Processing.

Recently, a huge set of systems, devoted to emotions recognition has been built, especially due to its application in many work domains, with the aims to understand human behaviour and to embody this knowledge into human-computer interaction or human-robot interaction [1]. The recognition of human expressions is a very complex problem for artificial systems, caused by the extreme elusiveness of the phenomenon that, starting from six basic emotions, creates a series of intermediate variations, difficult to recognize by an artificial system. Furthermore, the expression of the emotions has been simplified. Artificial systems are tuned on negative and positive emotions, so many times the recognition fails. To overcome these difficulties, and expand artificial knowledge, a Machine Learning (ML) system has been designed with the specific aim to develop a recognition system modelled on human cognitive functions. In particular, the code was developed in Mathematica [2] and organised in two steps: recognition of the 6 basic emotions and recognition of emotions in its different nuances in the same subject. Cohn-Kanade database images [3] was used precisely for the specifications of this data set. Subjects gradually express the six basic emotions from the onset of specific emotion (neutral expression) towards its peak, allowing the ML to recognise them even if produced by subjects from different perspectives and different levels. After training the ML, it was tested on a representative sample of unstructured data, acquired from social media. The results show a surprising progress in performance, compared to traditional systems, such as Azure and Watson.

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Algorithms for Jewelry Industry 4.0

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Keywords. algorithm for jewelry;computational desig,parametric jewelry.

This paper proposes a novel approach to improve the smart manufacture in jewelry industry 4.0 using parametric modeling systems that permits at the customers to modify the 3D virtual model. Parametric design systems model a design as a constrained collection of schemata (Aish,Woodbury, 2005) in the form of a graph named Direct Acyclic Graph (DAG). The 3D models of the jewels have been developed in Wolfram Mathematica® and Grasshopper software through a search of complex shape obtained from mathematical functions. The principal aim of designers has always been the development of a generative design system that applies affine transformations to original elements and create new 3D shapes based on a finite set of shape rules (Kielarova, et al. 2013). In this approach, designers define the geometry relationships and the constrains establishing the structure of the DAG. This allows to explore the design space when input parameters are changed in real-time. A generic DAG, grouped in a unit called User Object (Harding, Shepard, 2017), operates as a cognitive artifact shifting the focus from final form to the digital process (Oxman, 2005). Consequently, it can return countless and unique combinations so that the user can choose his preferred object. The object is ultimately physicalized via a 3D printer and used to build the final jewel. The latest version of prototype is made by wax-based resins that melt in low temperatures and it can be used in traditional goldsmith processes.

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Addition of Integers Embodied in Cellular Automata with Different Representations

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Keywords. Cellular Automata; Binary Representation; Integers Addition.

Diverse numeral representations can be embodied inside Cellular Automata (CA) for operating related operations. The CA calculation for the canonical representations doesn't involve significant time improvements if the operation is intrinsically sequential [1], while the CA parallelism could be completely exploited for the same operation with a redundant representations in a trade-off space/time [2]. The more efficient redundant representations are preferable if the computation result has not to be used in the canonical representations, because the translation "redundant/canonical", unlike the translation "canonical/redundant", has a computational cost that annuls the advantage. This research investigates such a problem for the addition of integer numbers, it is an extension of an analogous study related to the natural numbers [3]. Two 1–dimension CA with ring topology are considered: *cIadd*, performing addition of two addends in the conventional binary representation *cI* for integer numbers and *rIadd* performing addition in a redundant binary representation of integers *rI*, where a couple of binary digits shares the same positional weight. Relevant theorems about properties of both CA are demonstrated.

The worst case of computational cost for an addition in *cIadd* is given by l CA steps, where l is the *cIadd* number of cells. Computational cost for an addition of two addends n and m in *rIadd* is 2 *rIadd* steps, independently of the number of the CA cells. *rIadd* looks more efficient, if the results don't need to be produced in *cI*. The passage from redundant representation to the conventional one can be performed inside *rIadd* with a time cost of l step in the worst case. Such results demonstrate that computations involving long successions of operations based exclusively on additions can satisfactorily exploit the representation redundancy.

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Clustering analysis to profile customers behaviour in POWER CLOUD energy community

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Keywords. Machine learning; Cluster analysis; Consumer behaviour.

This paper presents a cluster analysis study on energy consumption dataset to profile "groups of customers" to whom address POWERCLOUD services. POWER CLOUD project (PON I&C2014-2020) aims to create an energy community where each consumer can become also energy producer (PROSUMER) and so exchange a surplus of energy produced by renewable sources with other users, or collectively purchase or sell wholesale energy. In this framework, an online questionnaire has been developed in order to collect data on consumers behaviour and their preferences. Together with demographic data, the most relevant information has been collected on home appliances and their actual power consumption, main sources of heating or cooling, the availability to adopt domotic solutions and in general, their availability to change their consumption profile according to renewable source. A clustering analysis was carried on the filled questionnaires using Wolfram Mathematica software, in particular FindClusters [1] function, to automatically group related segments of data. FindCluster function applies Machine Learning techniques to select and group homogeneous elements in a set of data to reduce the search space and to find the optimal solutions [2]. In our work, clustering analysis allowed to better understand the energy consumption propensity according the identified demographic variables. Thus, the outcomes highlight how the availability to adopt technologies to be used in PowerCloud energy community, increases with the growth of the family unit and, a greater propensity is major present in the age groups of 25-34 and 35-44.

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A symbolic model for infinitesimal calculus

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Keywords. Grossone; mathematics education; computer applications.

The knowledge and understanding of abstract concepts systematically occur in the studies of mathematics. The epistemological approach of these concepts gradually becomes of higher importance as the level of abstraction increase and the risk of developing a "primitive concept" which is different from the knowledge of the topic itself. A typical case relates to the concepts of infinity and infinitesimal. The basic idea is to overturn the normal "concept-model" approach: no longer a concept which has to be studied and modeled in a further moment but rather a model that can be manipulated (from the calculation point of view) and that has to be associated to a concept that is compatible with the calculus properties of the selected model. The goal is the ability to express a concept regardless of the intrinsic difficulties of the representation. The symbol for the infinite is in use "gross one" ($\sim$ "big one"). With this model based approach, the "symbol-concept" association overcomes operational limits of an inadequate language.

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A geometrical proof for generalized Goodstein's theorem

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Keywords. big data; goodstein; rooted trees.

Expressing a number as the sum of powers of some base b multiplied by digits $\in \{1, \ldots, b-1\}$ and recursively doing the same for the exponents involved in the sum leaves a notation where no number greater than b is involved, the so-called "hereditary base-b notation" which is considered in the statement of Goodstein's theorem (see [1]). Using a geometrical approach, one can turn these sums into a labeled rooted tree (see [2]) and give a more elementary and geometric proof for the aforementioned theorem. A more general version of the theorem can be stated (see [3]) and proved as well in this geometrical fashion. The simplification will allow us to better understand the underlying logical problems for the necessity of transfinite induction in the proof, as well as exploring other similar problems (for example, the "hydra game") and giving applications in the field of big data storage, where neural networks are indeed based on tree-like structures.

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A multi-factor RSA-like scheme with fast decryption based on Rédei rational functions over the Pell hyperbola

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Keywords. cryptography; Pell conic; Rédei rational functions; RSA.

RSA is one of the most widespread asymmetric encryption scheme. During the years, several attacks have been studied, like the Wiener attack, which is possible when the (private) decryption key is small, or the Coppersmith method, which can be exploited for small (public) encryption keys. Moreover, RSA shows some vulnerabilities in broadcast scenarios, i.e., when the same message is encrypted for different receivers using the same encryption key. Some variants of the RSA scheme have been proposed for obtaining cryptosystems that are not subjected to the above problems and having also a faster decryption procedure (which is usually the more time consuming task in RSA). In [1], the authors presented an RSA-like scheme based on Rédei rational functions, which are classical tools in number theory, over the Pell hyperbola, defined by $H = \{(x, y) \in \mathbf{R} \times \mathbf{R} : x^2 - Dy^2 = 1\}$, with $x^2 - D$ irreducible over $\mathbf{R}$, which can be equipped with the product

$$(x, y) \otimes (w, z) = (xw + yzD, yw + xz), \quad \forall (x, y),\ (w, z) \in H,$$

so that $(H, \otimes)$ is a group. Then, for the cryptographic application, the operations are performed in $\mathbf{Z}_N$, with N product of two primes, like in RSA. We see that this scheme can be also exploited when the modulus is a product of more than two primes or when $N = p^r q^s$, for p, q primes. In this way, the exponentiations (i.e., encryption and decryption of messages) can be performed exploiting the Chinese remainder theorem and the Hensel lifting method, greatly improving the decryption procedure. The proposed scheme appears to be more efficient than the analog ones constructed over elliptic curves, like the KMOV cryptosystem [2]. Moreover, our scheme is not subjected to impossible group operation attacks for large ciphertext size.

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Some results about n-sets

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Keywords. n-sets; divisor; multiple.

A result of a student of Erdős is well-know: for every integer $n \geq 1$, each subset of $I(2n) = \{1, 2, \ldots, n+1, n+2, \ldots, 2n\}$ having size $n+1$, contains at least two distinct elements of which the smallest divides the largest. This is proved using the pigeonhole principle. On the other side, it is easy to see that there are subsets of $I(2n)$ of size n without *divisor-multiple pairs*; we call them n-sets.

We give a precise description of elements that, for a fixed n, do not belong to every n-set, as well as elements that do belong to every n-set.

Furthermore, we give an algorithm to count n-sets, given n. In this way we can see the behavior of the sequence $a(n)$ of the number of n-sets. We will show some different version of the algorithm, along with their performances.

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The Carboncettus quasi-regular octagon and other polygons

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Keywords. Fibonacci numbers; golden ratio; irrational numbers.

In [1,3] G. Pirillo presented the audacious thesis that the first mathematicians who discovered the "so-called" Fibonacci numbers were some members of the Pythagorean School, well documented and active in Crotone in the 6th, 5th and 4th centuries B.C., hence more than 1,500 years before *Leonardo Pisano*, known as *"Fibonacci"*, wrote his famous *Liber Abaci* (1202). Such a thesis is mainly supported by computational evidences arising from pentagon and pentagram.

The paper [2], on the other hand, is centered on some geometric figures present on the sides of a portal of the cathedral of Prato (FI, Italy), which date back to around the middle of the 12th century (hence before the *Liber Abaci* as well) and should be works of *Carboncettus marmorarius*. The paper in question, that highlights the differences between the regular octagon and the one that has been named the *Carboncettus quasi-regular octagon*, likewise involves Fibonacci numbers and shows a beautiful symbolism typically medieval. Moreover, it has greatly stimulated many discussions and further investigations in different directions among the authors, and towards possible geometric generalizations both theoretically and numerically.
Finally, the importance of the octagonal shape in architecture and engineering will be also briefly discussed.

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The Arithmetic of Infinity within the continuum of enquiry: experiences in schools

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Keywords. Grossone; infinity; paradox; education; Dewey; enquiry.

As a rule, European mathematical curricula present school students with the notion of infinity in the context of the calculus. Infinity remains implicit in acquired techniques, e.g. differentiation, and becomes explicit when it proves a source of problems, e.g. when limits are hard to evaluate or certain calculations are forbidden. The introduction of infinity settles some problems and, at the same time, provides data for new ones. It is, in the terminology of [1], set within *the continuum of enquiry.* Nevertheless, the curricular aim to instil canonical intellectual habits usually abridges enquiry into the notion of infinity by imposing set bounds upon it. In this presentation we examine episodes from school workshops held in Italy and the UK, in which students were encouraged to overstep curricular bounds, reflect on straightforward issues posed by the calculus notion of infinity and, finally, consider and adopt new resources in order to tackle those issues. Typically, issues were highlighted by means of well-known paradoxes of infinity and new resources were taken from the framework of The Arithmetic of Infinity (AoI) described in [3], which was made available to students through simple exercises or a short presentation. Results (a preliminary discussion appears in [1]) show that students were often able to reinsert the notion of infinity within the continuum of enquiry and, when they did, they could also make insightful observations and personal discoveries.

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A computational approach with MATLAB software for nonlinear equation roots finding in High School Maths

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Keywords. Math Education; Iterative methods; MATLAB software.

Solving nonlinear equations is a part of the Maths syllabus of the experimental sections of the Italian secondary school for decades and is often present in the questions of the written test of the State Exams (National High School Examination). Despite its considerable relevance, in classroom teaching practice this subject is often overlooked or treated more from a theoretical than from a computational point of view. It is believed that this constitutes a serious gap in educational standards because the topic is understood in its essence only if various examples are resolved supported by mathematical software, and not by reducing it to a series of calculations, mostly by hand, often insignificant and detached from real contexts. The use of mathematical software not only supports an education of Applied Mathematics but at the same time provides teachers with tools and ideas conducive to engaging the students in activities-based learning of mathematics encouraging several aspects of maths - empirical, speculative, formal, and reflective.
This paper is part of the debate surrounding computer programming in the secondary school mathematics curriculum, with special focus on implementing algorithms related to appropriate methods for solving the nonlinear equation f(x)=0 with the use of MATLAB software. The aim is to favour the algorithm as a synthesis between the syntactic and semantic aspects of mathematical objects as well as encouraging computer simulation interpreted as a 'physical' experiment and a source of conjecture.

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A problem-solving approach to Diophantine equations in Math education contest

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Keywords. Bézout Theorem; Diophantine equations; Math education.

The search for integer solutions to a problem for which the mathematical model is a linear Diophantine equation $ax + by = c, \ a, b, c \in \mathbb{N}_0$ shows, on the one hand, how many situations requiring integer solutions are manifold and, on the other, it makes us understand how important it is to establish in which numerical set we look for solutions.

In the didactic practice of the Italian secondary school the Diophantine equations, in most cases, are not studied very much, in part because the textbooks devote little space to solvable problems or equations with integer solutions and a lot, instead, to the resolution of problems and equations in the set of real numbers. In those few cases where exercises are encountered in which students are asked to search for integer solutions, this never comes from a problematic situation. Consequently, there grows in students the conviction that an equation is solvable with on solution or non-solvable "in absolute".

This paper illustrates a practical, coherent example of problem-solving approach to linear Diophantine equations aimed at making students reason that such equations can admit more than one solution or even an infinite number of solutions. The aim is to favour the formulation of conjectures and the process of logical deduction (demonstration) to reach the resolution of a linear Diophantine equation, using the Euclidean algorithm for the calculation of the Greatest Common Divisor (GCD) of two or more integers which are not all zero, and the Bézout Theorem.

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Optimization and Management of Water Supply

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Numerical experimentations for a new set of local indices of a water network

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Keywords. Urban water supply systems; performance indices; network analysis.

Very recently in CaMa, a new set of local indices has been proposed for an urban water distribution network together with a useful mathematical framework that organizes and provides the tools to treat the complex of these local parameters varying from node to node. In this talk, the applicability of such indices to various models of both abstract and real hydraulic networks will be explored through direct numerical computations and hydraulic simulations. Furthermore, starting from explicit data sets for these local parameters and using the tools offered by the mentioned mathematical setting, some well known and very frequently used global energetic indicators will be calculated in a new way and through new formulas (for example, measures of resilience, pressure, deficiency, etc.).

Finally, since the tools and the framework proposed in CaMa have the important advantage of favoring in many cases a more in-depth structural analysis of global indices, new interpretations and new implications will be briefly discussed.

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A useful mathematical framework acting on a new set of local indices for urban water networks

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Keywords. Mathematical modeling; urban water networks; performance indices.

In recent years many authors have introduced, sometimes with considerable success, a multitude of indices, especially of energetic-hydraulic nature (for example, indices of resilience, robustness, pressure, failure, flow deficit, mechanical redundancy, balance, reliability, entropy, etc.), to characterize and summarize in a single parameter some of the most important peculiar characteristics of a complex water network (for a recent review of 21 different resilience measures see, for instance, [2]). Therefore these indices, which are expressly designed to be of global nature, do not adapt very well to local analysis even applying them to a small portion of the network (a small portion of a network, in fact, is not the same as a small independent network).

We propose here a new set of local indicators within a mathematical framework which is also unprecedented, as far as we know, for hydraulic-engineering purposes. Such indices, besides providing the basis for a local analysis of the water network, can be seen as the bricks with which, by means of the mathematical tools offered by the aforementioned setting, one can construct as many global indices as one wants, and naturally recover many of those already known, often also giving a deeper structural interpretation of the same (see [1] for details). This possibility, which will be explicitly illustrated in many cases during the talk, gives a strong automatic validation to the new proposed machinery.

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Identification of Contamination Potential Source (ICPS): a topological approach for the optimal recognition of sensitive nodes in a water distribution network

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Keywords. Water quality; contamination sources; graph theory.

The correct management of urban water networks have to supported by monitoring [1] and estimating water quality. The infrastructure maintenance status and the possible of a prevention plan availability influence the potential risk of contamination [2]. In this context, the Contamination Source Identification (CSI) models aim to identify the contamination source starting from the concentration values referring to the nodes [3]. This paper proposes a methodology based on Dynamics of Network Pollution (DNP). The DNP approach, linked to the pollution matrix [4] and the incidence matrix, allows a topological analysis on the network structure in order to identify the nodes and paths most sensitive to contamination, namely those that favor a more critical diffusion of the introduced contaminant. The procedure is proposed with the aim of optimally identifying the potential contamination points. By simulating the contamination of a synthetic network, using a bottom-up approach, an optimized procedure is defined to trace back to the chosen node as the most probable contamination source.

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Performance management of demand and pressure drive analysis in a monitored water distribution network

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Keywords. Water distribution network (WDN); pressure driven analysis (PDA) ; demand driven analysis (DDA).

The hydraulic modeling of the drinking water networks has been conditioned by the scarce availability of quality data but current technological advances can contribute to the improvement. In this context, the present work describes the research activity carried out in relation to the modeling aspects of drinking water networks in particular with referring to the simulation and calibration models. For this purpose, we have used WaterNetGen[1], an extension of the Epanet hydraulic simulation software. The EPANET simulation model assumes that water demand is always satisfied regardless of pressures (DDA)[2], indeed WaterNetGen associates a new solver (PDA)[3]. A comparison between the software outputs is the starting point for a new method of allocation and distribution of demand and water losses along the network, obtaining values closer to the measured data. The case study is the water distribution network of Nicotera (Italy).

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Optimization model for water distribution network planning in a realistic orographic framework

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Keywords. Optimization model; graph theory; water planning model.

Defining criteria for correct distribution of water resource is a common engineering problem. Stringent regulations on environmental impacts underline the need for sustainable management and planning of this resourceusage, which is sensitive to many parameters [1]. To manage optimally their number and variability are often used an optimization models. This work takes up and revises the minimum cost optimization model of a water distribution network with multiple supply sources andusers presented in [2] with the aim of overcoming the limits linked to the territory orographic complexity. In this direction, the model presented proposes an advancement of the optimization model, using the calculation of geodetic paths [3], compatible with hydraulic constraints. The method complexity is mainly linked to identifying geodetic pathways, which represents an intricate problem in computational and differential geometry. The application of the model is presented in a real case in Calabria.

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Seeking for a trade-off between accuracy and timeliness in meteo-hydrological modeling chains

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Keywords. hydro-meteorological modeling; warning lead time; weather mo-del resolution.

The level of detail achieved by operational General Circulation Models (e.g., the HRES 9 km resolution 10-day forecast recently launched by the ECMWF) raises questions about the most appropriate use of Limited Area Models, which provide for further dynamical downscaling of the weather variables. The two main objectives targeted in hydro-meteorological forecasts, i.e. accuracy and timeliness, are to some extent conflicting. Accuracy and precision of a forecast can be evaluated by proper statistical indices based on observations, while timeliness, once the calculation domain has been set, mainly depends on the spatial resolution of the grid and the computational resources used.

In this research a number of experiments is set up applying the Advanced Research Weather Research and Forecasting (WRF-ARW) Model [1] to two extreme weather events with different meteorological characteristics occurred in Southern Italy in 2016 and 2018 [2]. The accuracy of the forecast is evaluated both for the HRES ECMWF output and that provided by WRF dynamical downscaling at different resolutions. Furthermore, timeliness of the forecast is assessed adding to the time needed for GCM output availability the time needed for Limited Area simulations at different resolutions and using varying core numbers.

The research provides useful insigths for operational forecast in the study area, highlighting the level of detail required and the current weaknesses hindering correct forecast of the hydrological impact of extreme weather events.

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Scenario optimization in complex water supply systems for energy saving and a correct management under uncertainty

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Keywords. Energy optimization; Water management; Scenario analysis; Cost-risk balancing approach.

The management of complex water supply systems needs a close attention to economic aspects concerning high costs related to energetic management [4]. Specifically, the optimization of water pumping plants activation schedules is an important issue, especially managing strategic and costly water transfers under drought risk [1]. In such management context and under uncertainty conditions, it is crucial to assure simultaneously energy savings and water shortage risk alleviating measures. The model formulation needs to highlight these requirements duality: to guarantee an adequate water demands fulfilment respecting an energy saving policy. This modelling approach has been developed using a two stages scenario analysis [3] with a cost-risk balancing approach [2], achieving simultaneously an energetic and operative costs minimization and assuring an adequate water demand level fulfilment for users. This model has been implemented using the software GAMS interfaced with CPLEX solvers. An application of the proposed optimization approach has been tested considering the draft of a real supply system located in a drought-prone area in North-Sardinia (Italy). By applying the optimization procedure, a robust decision strategy in pumping activation was obtained considering this real case study.

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Optimizing rainwater harvesting systems for non-potable water uses and surface runoff mitigation

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Keywords. Rainwater harvesting; water supply; flood risk mitigation.

Rainwater harvesting (RWH) systems represent sustainable solutions which meet the challenges of water saving and surface runoff mitigation. The collected rainwater can be re-used for several purposes irrigation of green roofs and garden, flushing toilets, etc. Optimizing the water usage in each section is a significant factor and, therefore, in the current paper was considered.

To achieve this goal different methods for Multi-Objective Optimization can be considered. The ranking methods such as TOPSIS (Technique for Order Preference by Similarity to Ideal Solution) can be used for comparing algorithms and to evaluate the performance of alternatives to reach to the ideal solution. The results of ranking methods such as TOPSIS or multiple attributes decision-making methods such as Rough Set method can increase the efficiency and reduce the cost of project by preventing uncertainties. Moreover, the analysis by Rough Set method not only can provide a baseline for decision making but also insights to the problem of concern.

In conclusion, the numerical optimization of RWH systems will improve the previous studies in the field, and provide an additional tool to identify the optimal rainwater reuse in order to save water and reduce the surface runoff discharged into the sewer system.

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New Mathematical Optimization Approaches for LID Systems under Fuzzy Environment

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Keywords. Optimization; LID; Rough Set theory.

The urbanization affects the ecosystem health and downstream communities by changing the natural flow regime. In this context, Low impact development (LID) systems are important tools in sustainable development.

There are many components in design and operation of the LID systems and even choosing the selected LID and the location of that in the basin can affect the results. In this regards, the Mathematical Optimization Approaches can be used as an ideal method to optimize the use of LIDs. In the current research, the application of TOPSIS (Technique for Order Preference by Similarity to Ideal Solution) and Rough Set theory (multiple attributes decision-making method) was considered. One of the advantages of using the Rough Set method in LID systems is that the selected decisions are explicit and method is not limited to restrictive assumptions.

The new presented mathematical optimization approaches for LID systems under fuzzy environment will improve the previous studies in this subject and will provide engineers an additional valuable tool in analyzing essential attributes to select and optimized the best LID system for the project.

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Evaluation of an integrated seasonal forecast system for agricultural water management in Mediterranean regions

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Keywords. meteo-hydrological system; seasonal forecast; agricultural water management.

The Euro-Mediterranean Center on Climate Change (CMCC) seasonal forecasting system [1] is conceived and run in Italy and is based on the global coupled model CMCC-CM. The seasonal predictions are performed every month, producing a number of ensemble integrations conducted for the following 6 months. In this study, a performance evaluation of the skills of this system is performed in two neighbouring Mediterranean medium-small size basins located in Southern Italy, the Crati River and the Coscile River, whose hydrological cycles are particularly important for agricultural purposes.

Initially, the performance of the system is evaluated in terms of agreement both between observed and simulated precipitation and temperature anomalies and the associated large scale signals (composites of 500hPa geopotential height, MSLP and winds), in the irrigation periods of the years 2011-2017. Forecasts issued on April 1st (i.e., at the beginning of the irrigation period) are evaluated, considering two lead times (first and second trimester).

Afterward, the seasonal forecasts are integrated in a complete meteo-hydro-logical system. Precipitation and temperature anomalies provided by the global model are ingested in the spatially distributed and physically based In-STRHyM (Intermediate Space-Time Resolution Hydrological Model) model [2], which analyzes the hydrological impact of the seasonal forecasts.

The integrated seasonal forecast system showed to provide useful and timely indications for agricultural water management in the study area.

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Optimization of submarine outfalls with a multiport diffuser design

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Keywords. Sea water quality; submarine outfalls; optimization design.

Immission of civil sewage into the sea is realized to complete the depurative onshore process or to take out from the bathing area the already purified wastewater, ensuring a good perceived seawater quality [1]. Anyhow the compliance of the pollutants concentration limits is necessary to ensure safe bathing. The design of submarine pipes is usually completed contemplating a diffuser with a series of vents for the repartition of the wastewater discharge [2]. The real process of pollutants diffusion into the sea, simulated with complex diffusion-dispersion models in a motion field dependent from environmental conditions and drift speeds, affect the submarine pipe design [3]. An optimization procedure has been realized for the marine outfall pipe-diffuser system using a simplified zone model [4], subjected to a sensitivity analysis on the characteristic parameter. The method is shown using an example project for the submarine outfall at service for the sewage treatment plant of Belvedere Marittimo, on the southern Tyrrhenian Sea in Italy.

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Computational Methods for Data Analysis

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Exact and Approximate Analytical Solutions for Nonlinearly Colloid Facilitated Solute Transport

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Keywords: nonlinear transport; colloids; analytical solutions.

Colloid facilitated solute transport in homogeneous porous media is investigated. Sorption on the matrix is modelled by the linear equilibrium isotherm whereas sorption on colloidal sites is regulated by nonlinearly equilibrium and nonequilibrium [3, 2]. Two equilibrium isotherms describing sorption on colloidal particles are considered, that is, Langmuir and Freundlich equations [1]. Exact analytical solutions for equilibrium are obtained and discussed in order to asses the impact of nonlinearly sorption. Travelling wave analytical solutions are obtained to describe the evolution in both the liquid and colloidal concentration. Besides expressions for the front shape, the mathematical shape of the front thickness and the front positions are also presented.

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Performance analysis of a multicore implementation for solving a two-dimensional inverse anomalous diffusion problem

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Keywords. Fractional models; Multicore architecture; parallel algorithms.

In recent decades, fractional calculus has become highly attractive due to wide applications in science and engineering. Indeed, fractional models are beneficial and powerful mathematical tools to describe the inherent properties of processes in mechanics, chemistry, physics, and other sciences. Meshless methods represent a good technique for solving these models in high-dimensional and complicated computational domains. In particular, in the current work we deal with the solution of a two-dimensional inverse time fractional diffusion equation, involving a Caputo fractional derivative in his expression, using a sequential approach described in [1, 2]. Since we deal with a huge practical problem with a large domain, by starting from an accurate meshless localized collocation method using RBFs, here we propose a fast algorithm, implemented in a multicore architecture, which exploits suitable parallel computational kernels. More in detail, we firstly developed, a C code based on the numerical library LAPACK to perform the basic linear algebra operations and to solve linear systems, then, due to the high computational complexity, when real datasets are considered, we propose a parallel algorithm specifically designed for multicore architectures and based on the Pthreads library. An easy-to-use interface makes possible to vary both the main parameters of the problem and the threads number. Experimental results together with a suitable performance analysis will prove the reliability and the efficiency of the developed algorithm. The performance gain is measured in terms of execution times, speed-up, efficiency and scalability.

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Stochastic Mechanisms of Information Flow in Phosphate Economy of *Escheria Coli*

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Keywords. synthetic biology; *E. coli*; modelling, stochasticity.

The rapidly growing field of synthetic biology, at the crossroads of molecular biology, genetics and quantitative sciences, aims at developing living technologies by re-engineering the make-up of organisms. The applications in this field are designed by channeling the quantitative understanding of the molecular processes to a methodological workflow that can be compared to the use of mechanics in civil engineering. The aim, in these applications, is to modify the organisms to enhance and benefit from their natural capacity for certain tasks. For example, in enhanced biological phosphorus removal (EBPR) micro-organisms such as *E. coli* are used to profit from their inherent regulatory mechanisms that efficiently respond to phosphate starvation. In previous work, we have presented a computational model and experimental results that quantify the dynamic mechanisms of auto-regulation in *E. coli* in response to varying external phosphate levels [1]. In a cycle of deterministic ODE simulations and experimental verification, our model predicts and explores phenotypes with various modifications at the genetic level that can optimise inorganic phosphate intake. Here, we extend our analysis with extensive stochastic simulations at a single-cell level so that noise due to small numbers of certain molecules, e.g., genetic material, can be better observed. For the simulations, we resort to a conservative extension of Gillespie's stochastic simulation algorithm that can be used to quantify the information flow in the biochemical system besides the common time series analysis [2, 3]. We argue that our stochastic analysis of information flow provides insights for designing more stable synthetic applications that are not affected by noise.

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Adaptive RBF Interpolation for Estimating Missing Values in Geographical Big Data

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Keywords. Big data analysis; Data imputation; RBF interpolation; SVM.

The quality of datasets is a critical issue in big data mining. More interesting things could be found for datasets with higher quality. The existence of missing values in geographical big data would worsen the quality of big datasets. To improve the data quality, the missing values are generally needed to be estimated using various machine learning algorithms such as the Support Vector Machine (SVM) or mathematical methods such as approximations and interpolations [1-2]. In this paper, we propose an adaptive Radial Basis Function (RBF) interpolation algorithm for estimating missing values in geographical big data. In the proposed method, the samples with known values are considered as the data points, while the samples with missing values are considered as the interpolated points. For each interpolated point, first, a local set of data points are adaptively determined. Then, the missing value of the interpolated point is imputed via interpolating using the RBF interpolation based on the local set of data points. Moreover, the shape factors of the RBF are also adaptively determined by considering the distribution of the local set of data points. To evaluate the performance of the proposed method, we compare our method with the commonly used SVM, and conduct three groups of benchmark experiments. Experimental results indicate that the proposed method outperforms the SVM for irregularly distributed datasets, but worse than the SVM for regularly distributed datasets.

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Data-based models for satellite images

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Keywords. Kernel-based interpolation, Caratheodory-Tchakaloff compression, Padova points.

Exploitation of the huge amount of spatially distributed data via model simulation needs model reduction schemes to be able to deliver the sought services such as, e.g., short term real-time predictions, feature extraction, data comparison.

Effective synthesis via data-based modeling can be achieved only via suitable reduced order models that must be at the same time robust and provide controlled accuracy to ensure meaningful analysis of the variables of interest.

More specifically, we focus on two aspects of data-based modeling:

- Compression: reduce the number of sampling points in the reconstruction of satellite images via Caratheodory-Tchakaloff or Padova points subsampling; see e.g. [1, 3].
- Reconstruction: accurately approximate the image via polynomial least squares or discontinuous kernel-based methods [2], using the compressed sampling points.

After providing a theoretical framework, we extensively test the proposed techniques on satellite images consisting of raw data by NASA Soil Moisture Active Passive (SMAP) satellite and simulated data obtained via the TERRestrial SYStem Modelling Platform (TerrSysMP).

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Approximate leave-one-out cross-validation for nonparametric Bayesian Gaussian Process methods with applications to neural data

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Keywords. Scalability; Nonparametric Bayesian; Gaussian Processes; Generalized linear models; Laplace approximation; Neural data.

Recently, we developed a scalable methodology called approximate leave-one-out (ALO) as a computationally efficient alternative to the time-consuming and memory demanding leave-one-out cross-validation (LO) [Rahnama Rad and Maleki, 2019]. ALO uses all the data, estimates the model only once, and using an analytical approximation computes LO without repeatedly leaving a datum out and estimating the model again. In addition to obtaining the model estimate, ALO requires a matrix inversion and two matrix-matrix multiplications. Despite these extra steps ALO offers a significant computational saving compared to LO.

The ALO methodology was specifically innovated for point estimates of penalized generalized linear models. In this abstract we propose an extension of the ALO methodology for the tuning of hyper-parameters in Bayesian models. In our examples, we focus on Gaussian process nonparametric Bayesian techniques for spatio-temporal point process data. The computational efficiency of our algorithm is based on fast sparse matrix vector multiplications, low-rank updates, and the conjugate gradient method [Rahnama Rad et al., 2017]. The log-concavity of the posterior and the Laplace approximation provide further analytical simplifications [Rahnama Rad and Paninski, 2010]. Finally, we illustrate the computational efficiency and statistical robustness of this methodology by applying it to novel experimental data from the entorhinal cortex, a region of the brain involved in spatial navigation [Hafting et al. 2005].

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Numerical approach for NMR-based analysis of water mobility in wheat flour dough

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Keywords. Bread making; Dough; Laplace transform.

The understanding of the breadmaking process requires to understand the changes in water mobility of dough. The dough ingredients as well as the processing conditions determine the structure of baked products which in turn is responsible for their apparence, texture, taste and stability. The transition from wheat flour to dough is a complex process in which several transformations take place, including those associated with changes in water distribution [1]. The molecular mobility of water in foods can be studied with proton nuclear magnetic resonance (1H NMR). Low-resolution (LR) 1H NMR has been mainly used to measure the transverse relaxation times (T2) in dough and bread [2]. In this study, the measured T2 was used to investigate wheat dough development during mixing. The interactions of the flour polymers with water during mixing reduce water mobility and result in different molecular mobilities in dough. The molecular dynamics in heterogeneous systems are very complex. From a mathematical point of view the NMR relaxation decay is generally medelled by the linear superposition of a few exponential functions of the relaxation times. This could be a too rough model and the classical fitting approaches could fail to describe physical reality. A more appealing procedure consists in describing the NMR relaxation decay in integral form by the Laplace transform (LT) [3]. In this work an algorithm for the LT inversion is considered and compared with other classical numerical techniques.

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First Order Methods in Optimization: Theory and Applications

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Proximal Approaches for Matrix Estimation Problems

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Keywords. Matrix Estimation, Non–convex Optimization, Graphical Lasso

In recent years, there has been a growing interest in problems such as graph estimation, gene expression, brain network analysis, computer vision: the mathematical formulation of such applications leads to the minimization of a Bregman distance [1] coupled with a regularization term. The variational models describing the above problems usually involve convex functionals, but some practical applications actually require concave ones. We propose two strategies, in order to address both the convex and the non–convex case.

The first approach consists in splitting the regularization functional in two terms, one being a spectral function while the other is arbitrary: a Douglas–Rachford approach [2] is proposed to address such problems and several options for the fit–to–data functional and for the regularization term are considered, providing a list of proximity operators. The second strategy minimizes non–convex problems via a majorization–minimization technique [3], i.e. modifying the original objective function with a convex approximation and solving the inner subproblems via the aforementioned Douglas–Rachford algorithm. Each proposed technique is numerically tested, in comparison with state–of–the–art algorithms [4]: the achieved results are very promising and competitive.

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A Neural Network Approach for Parameters Estimation in Image Deblurring

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Keywords. Image restoration; neural network; forward-backward algorithm.

Image deblurring is a well-known problem usually faced by means of a reformulation as an optimization problem, in which the objective function to be minimized is made up by a data discrepancy measure plus a regularization term, with the possible imposition of contraints to reduce the feasible set and incorporate a priori knowledge on the desired solution. According to the mathematical properties of the several terms (e.g, convexity, smoothness, contraints form), suitable numerical optimization methods have to be adopted to perform the minimization step.

In this talk we consider smooth data-fidelity and regularization functionals and we include the constraints in the objective function by means of a logarithmic barrier. A proximal interior point method (IPM) is adopted to address the minimization step [3], in which the proximity operator is restricted only to the barrier function. The key issue of our proposed approach is that the regularization parameter, the barrier parameters and the steplengths needed in the iterations of the IPM are chosen by exploiting suitable deep learning strategies [4].

We used benchmarks image datasets to train the neural networks architectures and test our approach. Comparisons with standard gradient projection methods and recent machine learning based algorithm have been performed and showed encouraging performances.

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Learning the Invisible: Limited Angle Tomography, Shearlets and Deep Learning

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Keywords. Deep neural networks; limited angle CT; shearlets; sparse regularization; wavefront set.

Limited angle geometry is still a rather challenging modality in computed tomography (CT), in which entire boundary sections are not captured in the measurements making the reconstruction a severly ill-posed inverse problem. Compared to the standard filtered back-projection, iterative regularization-based methods help in removing artifacts but still cannot deliver satisfactory reconstructions. Based on the result that limited tomographic data sets reveal parts of the wavefront (WF) set in a stable way and artifacts from limited angle CT have directional properties [3], we propose a hybrid reconstruction framework that combines model-based sparse regularization with data-driven deep learning. The core idea is to solve the compressed sensing formulation associated to the limited angle CT problem to recover the so called "visible" part of WF and learning via a convolutional neural network architecture the "invisble" ones, which provably cannot be handled by model-based methods [1]. Such a decomposition into visible and invisible parts is achieved using the shearlet transform that allows to resolve WF sets in the phase space [2]. Our numerical experiments show that our approach surpasses both pure model- and more data-based reconstruction methods, while offering an (heuristic) understanding of why the method works, providing a more reliable approach especially for medical applications.

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Barzilai-Borwein rules in gradient projection methods: a redefinition for special constrained problems

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Keywords. steplength selection; gradient projection method; variable metric.

Starting from the pioneering paper by Barzilai and Borwein (BB), which opened the way to inexpensively accelerate first-order methods, in the last decades several efficient steplength techniques (see [1,2] and the references therein) have been designed in order to make gradient descent methods more and more effective also for problems which handle large-scale data and require real-time solutions. In a very recent paper [4], the authors proved that, for quadratic programs, the spectral properties of the original BB schemes are affected by the presence of box constraints. In this talk we analyze how, in quadratic and non-quadratic minimization problems, the presence of a more general feasible region, expressed by a single linear equality constraint together with lower and upper bounds, influences the spectral behaviour of the BB-based rules employed in classical and variable metric gradient projection methods [3]. Moreover, on a set of test problems arising also from data mining applications, we numerically verify the benefits which can be gained by taking into account this influence in a new BB approach able to capture not only second order information but also the nature of the feasible set.

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Augmented Lagrangians with adaptive augmentation for bound and equality constrained quadratic programming problems

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Keywords. quadratic programming; augmented Lagrangians; bound and equality constraints.

Augmented Lagrangian method combined with effective algorithms for the solution bound constrained problems can solve efficiently very large QP problems with bound and equality constraints. Here we are interested in improvement of the SMALBE-M algorithm (semi-monotonic augmented Lagrangian for bound and equality constrained problems) [1, 2] which was a key ingredient of in a sense optimal algorithms for the solution of large (billions of nodal variables) discretized variational inequalities [4]. Recall that these algorithms can solve large discretized problems with asymptotically linear complexity [1, 2, 4].

The point of this lecture is to show that the performance of SMALBE-M can be essentially improved by plugging in the information on the active set from the current iterate by means of adaptive augmentation. The idea is related to the earlier experiments with adaptive projectors [3]. The improvement is demonstrated by solving large problems arising from the application of domain decomposition methods to the solution of elliptic variational inequalities.

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On the steplenght selection in Stochastic Gradient Methods

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Keywords. Stochastic optimization; stochastic gradient methods; steplenght selection; Barzilai-Borwein rules; limited memory strategies.

Many machine learning methodologies, based on the minimization of the empirical risk, lead to optimization problems in which the objective function is the sum of loss functions, depending on the samples of a finite training set. These optimization problems are challenging in the case of large scale training sets because the computation of the objective function and its gradient is too expensive. In these cases, Stochastic Gradient (SG) methods [1] are the main approaches. Many SG variants are available in literature, based on different strategies for reducing the adverse effect of noisy gradient estimates and for defining the steplength (or learning rate) parameter. In this work, starting from recent advances on state of the art steplength rules for deterministic gradient schemes [2] and noise reduction strategies, we investigate possible techniques for selecting the learning rate parameter in SG approaches. Preliminary studies on the behaviour of popular steplength selections, such as the Barzilai-Borwein rules, in the stochastic gradient framework, have shown that many interesting questions need to be fixed before obtaining effective benefits [4]. In this work, we investigate the possibility to make the SG algorithms more robust by exploiting steplength selections based on recently proposed limited memory strategies [3]. We also discuss some of these open problems on the steplength selection within other widely used stochastic optimizers, exploiting momentum terms and adaptive variance techniques.

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Adapting MPRGP Algorithm For Supervised Modelling of Biochemical Activities Employing SVM Classification

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Keywords. MPRGP; active-set method; SVM; chemogenomics;

Supervised modelling is widely used in the pharmaceutical industry, especially during the early stage of drug design and development. The aim is to train a model that generalizes biological activities of chemical compounds by reusing information from former laboratory experiments. Despite the fact that Deep Learning (DL) is getting popular in recent years, the Support Vector Machines (SVMs) are still applicable. Unlike the DL underlying architecture, SVMs could be considered as the single perceptron problems that find the learning functions that maximize the geometric margin between classes. Therefore, we can simply explain the qualities of a learning model and an underlying solver behaviour.

Our presentation deals with adapting the MPRPGP (Modified Proportioning with Reduced Gradient Projection), for the QP problems arising from the application of SVM formulations to the analysis of chemogenomics datasets. The MPRGP is an active-set method for solving the QP problems with bound or box constraints. For improving the convergence rate, we exploit the special structure of the dual QP-SVM. We are going to demonstrate the impact of an adaptive step-size in the expansion of an active-set. Numerical results obtained with different hinge-loss functions, a technique for calibrating a classification model, various performance scores, and binarization strategies will be presented as well.

Acknowledgements.

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Convergence of an inexact forward–backward method for nonconvex nonsmooth problems

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Keywords. Forward–backward algorithm; nonconvex optimization; image restoration.

We consider a general inexact forward–backward (FB) algorithm suited for minimizing the sum of a continuously differentiable function and a lower semicontinuous, convex term. The proposed scheme introduces an error into the computation of the proximal operator, by means of an implementable inexactness criterion, and combines a variable metric in the FB step with a linesearch procedure along the feasible direction [2]. Recently, the convergence of the considered scheme has been proved without any convexity assumption on the differentiable term, by requiring that the objective function satisfies the so-called Kurdyka–Łojasiewicz (KL) inequality; however, the result is given only with exact proximal evaluations [1]. We fill the gap in the convergence analysis of the algorithm under the KL assumption by proving the convergence of the iterates sequence, as well as the rates for the function values, when the proximal operator is computed inexactly. To this aim, we exploit the notion of forward–backward envelope [3] to define a continuously differentiable surrogate function, which satisfies the KL property on its domain, has the same value of the objective function at each of its stationary points, and complies with a certain relative error condition which allows to prove convergence in the KL framework. Furthermore, we apply the proposed inexact FB scheme to the restoration of blurred images corrupted by Cauchy noise, and show the numerical improvements obtained by introducing a variable metric into the computation of the FB step.

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A gradient-based globalization strategy for the Newton method

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Keywords. Newton method; global convergence; spectral gradient methods.

The Newton method is one of the most powerful methods for the solution of smooth unconstrained optimization problems. It has quadratic local convergence in a neighborhood of a local minimum where the Hessian is positive definite and Lipschitz continuous [1]. Several strategies have been proposed in order to achieve global convergence. They are mainly based either on the modification of the Hessian together with a line search or on the adoption of a restricted-step strategy [2].

We propose a globalization technique that combines the Newton and gradient directions, producing a descent direction on which a backtracking Armijo line search is performed. Our work is motivated by the effectiveness of gradient methods using suitable spectral step-length selection rules [3]. We prove global convergence of the resulting algorithm, and quadratic rate of convergence under suitable second-order optimality conditions. A numerical comparison with a modified Newton method exploiting Hessian modifications [4] shows the effectiveness of our approach.

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High Performance Computing in Modelling and Simulation

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A parallel software platform for pathway enrichment

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Keywords. Pathways; KEGG; REACTOME; Parallel computing.

Biological pathways are complex network models [1] able to provide a view on the interactions among bio-molecules inside the cell. Biological pathways are represented as a network, where the nodes are the bio-molecules, and the arches represent the interactions between two biomolecules.

All available information regarding the pathways are collected in several online repositories of pathways information such as KEGG [2] is a repository of metabolic pathways, Panther [3] comprises primarily signaling pathways, and Reactome [4] that contains information about metabolism and signal transduction pathways, to name few.

Pathways enrichment analysis is employed to help the researcher to discriminate relevant proteins involved in the development of both simple and complex diseases. To support the researcher to perform pathways enrichment analysis, several software tools are available. The main limitation of the current enrichment tools are: *i*) each tool can use only a single pathway source to compute the enrichment; *ii*) researcher have to repeat the enrichment analysis several times with different tools (able to get pathway data from complementary data sources); *iii*) enrichment results have to be manually merged by the user, a tedious and error-prone task even for a computer scientist. As a result, we propose a parallel enrichment tool able to retrieve at the same time pathways information from KEGG, Reactome, and Panther databases, with which to automatically perform pathway enrichment analysis, allowing to reduce the computational time of some order of magnitude, as well as the automatic merging of the results.

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Improving Efficiency in Parallel Computing Leveraging Local Synchronization

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Keywords. Parallel Computing, Speedup, Synchronization, Max-Plus Algebra.

In parallel computing, a complex task is typically split among many computing resources, which are engaged to perform portions of such task in a parallel fashion. Except for a very limited class of application, computing resources need to coordinate with each other in order to carry out the parallel execution in a consist way. As a consequence, a synchronization overhead arises [1], which can significantly impair the overall execution performance. Typically, the synchronization is achieved by adopting a centralized synchronization barrier involving all the computing resources. In many application domains, though, such kind of global synchronization can be relaxed and a lean synchronization schema, namely local synchronization [2], can exploited. By using local synchronization, each computing resource needs to synchronize only with a subset of the other computing resources.

In this work, we evaluate the performance of the local synchronization mechanism when compared to the global synchronization scenario. As a key performance indicator, the efficiency index is considered, which is the speedup normalized with respect to the number of computing nodes. The efficiency trend is evaluated both analytically and through numerical simulation. More in particular, the analytical study is carried out by exploiting extreme value theory [3] for the case of global synchronization, whereas, the max-plus algebra theory [4] is used in the case of local synchronization.

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A General Formalism for Multidimensional Space-Time Discrete Structured Grid Modelling

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Keywords. Structured Grid Modelling, Multidimensional space partitioning, Local and global transition rule, Aggregation and Disaggregation function, Parallel Computing.

Computational structured grids are often adopted in the simulation of complex systems, since they offer a good trade off between accuracy and efficiency [1]. Different formal models have been proposed in Literature to describe the computational process on the grid, such as Extended Cellular Automata [1] and Cellular Automata Neworks [3]. Here we propose a new formalism called *Structure+* with the aim of modeling multidimensional space-time discrete complex systems by means of one or more structured grids, each one with its own dimensionality and dimension. Both local and global transition rules can be defined to permit the different grids to evolve. Interface operators, like aggregation and disaggregation functions, can also be defined to allow the different domains to communicate and synchronize. A first example of a coupled surface to groundwater hydrological model is presented. Considerations about parallel computational aspects are eventually discussed.

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Preliminary model of saturated flow using Cellular Automata

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Keywords. High-performance Computing; Extended Cellular Automata; Computational Fluid Dynamics.

A fully-coupled from surface to groundwater hydrological model is being developed based on the Extended Cellular Automata formalism (XCA) [1], which proves to be very suitable for high performance computing. In this note, the module related to three-dimensional saturated flow in porous media is presented by using the OpenCAL library [2], allowing to exploit multi-core CPUs and many-core devices like GPUs. The XCA-based model is evaluated in terms of both accuracy and precision of modeling results and computational performance, using two- and three-dimensional test cases at different resolutions (from parcel to catchment scale), simulating pumping from one or more wells, river-groundwater interactions and varying soil hydraulic properties. Model accuracy is compared with analytic solutions, when available, and with the widely used MODFLOW model [3], while the computational performance is evaluated using both CPU and GPU devices. Overall, the XCA-based model proves to be accurate and, mainly, computationally very efficient thanks to the many options and tools available with the OpenCAL library.

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A cybersecurity framework for classifying non stationary data streams exploiting genetic programming and ensemble learning

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Keywords. Genetic Programming, Cybersecurity, Data streams.

The problem of classifying attacks in the cybersecurity field involves many issues, such as the need of dealing with fast data streams, the non-stationary nature of attacks (concept drift) and the uneven distribution of the classes. Classical data mining algorithms usually are not able to handle all these issues. Ensemble-based algorithms [2] fit well this challenging scenario, as they are incremental, robust to noise, scalable and operate well on unbalanced datasets. However, a clever and not computationally expensive strategy has to be designed to combine the classifiers composing the ensemble.

To this aim, a distributed genetic programming (GP) tool [1] is used to generate the combiner function of an ensemble; this tool does not need an heavy additional phase of training, after the classifiers composing the ensemble are trained, and, therefore, it can answer quickly to concept drifts, also in the case of fast-changing data streams. The above-described approach is integrated into a novel cybersecurity framework used for classifying non stationary and unbalanced data streams. This framework provides several drift detection functions and a strategy for replacing classifiers, which permits to build the ensemble in an incremental way. The architecture of the framework includes also a preprocessing module to extract and select data and context features and some repositories maintaining the discovered alerts and models.

We conducted experiments on artificial and real datasets and the framework is effective both in detecting attacks and in quickly reacting to concept drifts.

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Neural word embeddings approach for a distributed management system in healthcare

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Keywords. Neural word embeddings, Electronic Health Records, Semantic overlay network, Self-organization.

Today's health domain is characterized by heterogeneous, numerous, highly dynamics and geographically distributed information sources. Moreover, the increasing use of electronic health records (EHRs) has led to store an unprecedented amount of information. Managing this large amount of data can, often, introduce issues of information overload, with potential negative consequences on clinical work, such as errors of omission, delays, and overall patient safety [2]. Innovative techniques, approaches and infrastructures are needed to investigate data featured by high velocity, volume and variability. This paper introduces a distributed and self-organizing algorithm for building a management system for big data in highly dynamic environments like healthcare domain. EHRs and social data are represented with vectors obtained through the *doc2vec* model [1], a neural approach able to capture the semantic context representing documents in dense vectors namely *neural word embeddings*. Doc2vec is an unsupervised algorithm to generate vectors starting from sentences/documents based on *word2vec* approach which can generate vectors for words. Thanks to autonomous and local operations performed by the servers of a clinical distributed system, a logically organized overlay network emerges and the resource management operations become faster and efficient. Preliminary experimental results show the effectiveness of our approach.

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A Dynamic Load Balancing technique for Parallel Execution of Structured Grid Models

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Keywords. Parallel Computing, Parallel Software Tools, Load Balancing, Cellular Automata.

The distribution of computational load over different processing elements represents an important issue in parallel computing [1]. This is particularly relevant in the case of parallel execution of structured grid computational models, such as Cellular Automata (CA) [2], where the domain space is partitioned in region assigned to the parallel computing nodes. Load balancing techniques are particularly effective when structured grid computational models are exploited to simulate topologically connected physical phenomena like lava or debris flows (e.g., [3]), in which the evolution develops in a usually small sub-region of the domain. In this work, we present a dynamic load balancing technique that can provide performance improvements in structured grid model development on distributed memory architectures by adopting the MPI technology. First tests have demonstrated the usefulness of the feature in appreciably reducing execution times in comparison with not-balanced parallel versions.

Acknowledgements. Authors thank Rodolfo Calabrò from University of Calabria for helping in code implementation and testing phases.

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Final Sediment Outcome from Meteorological Flood Events: a Multi-Modelling Approach

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Keywords. Extreme Event; Flood; Sediment Transport and Deposition; Subaerial and Subaqueous Flow-like landslide; Modelling and Simulation.

Coastal areas are more and more exposed to the effects of climatic change. Intense local rainfalls increases the frequency of flash floods and/or flow-like subaerial and afterwards submarine landslides. The overall phenomenon of flash flood is complex and involves different phases strongly connected: heavy precipitations in a short period of time, soil erosion, fan deltas forming at mouth and hyperpycnal flows and/or landslides occurrence. Such interrelated phases were separately modelled for simulation purposes by different computational models: PDE methods for weather forecasts and sediment production estimation [1], Cellular Automata (CA) for soil erosion by rainfall and "subaerial" sediment transport and deposit [4], the behavior in the earth/sea interface and subsequent submarine flow may be modelled by the CA model SCIDDICA. This research studies the coupling of these models and introduces in SCIDDICA the process concerning the interaction currents/subaqueous sediments. A first validation of SCIDDICA in simple cases of submarine current/sediment interaction looks satisfying. Our aim is to complete the model and validate it on the 2016 Bagnara case [1], whose data [2] are sufficient for a complete simulation.

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Parallel Algorithms for Multifractal Analysis of River Networks

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Keywords. Multifractal dimension; River networks; Parallel algorithms.

The dynamical properties of many natural phenomena can be related to their support fractal dimension. A relevant example is the connection between flood peaks produced in a river basin, as observed in flood hydrographs, and the multi-fractal spectrum of the river itself, according to the Multifractal Instantaneous Unit Hydrograph (MIUH) theory. Typically, the multifractal analysis of river networks is carried out by sampling large collections of points belonging to the river basin and analyzing the fractal dimensions and the Lipschitz-Hölder exponents of singularities through numerical procedures which involve different degrees of accuracy in the assessment of such quantities through different methods (box-counting techniques, the generalized correlation integral method by Pawelzik and Schuster (1987), the fixed-mass algorithms by Badii and Politi (1985), being some relevant examples).

However, the higher accuracy in the determination of the fractal dimensions requires considerably higher computational times. For this reason, we recently developed a parallel version of some of the cited multifractal methods described above by using the MPI parallel library, by reaching almost optimal speed-ups in the computations. This will supply a tool for the assessment of the fractal dimensions of river networks (as well as of several other natural phenomena whose embedding dimension is 2 or 3) on massively parallel clusters or multi-core workstations.

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A methodology approach to compare performance of parallel programming models on HPC applications

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Keywords. MPI; OpenMP; NUMA; HPC; Parallel programming patterns.

The majority of current HPC applications are composed of complex and irregular data structures that involve techniques such as linear algebra, graph algorithms, and resource management, for which new platforms with varying computation-unit capacity and features are required. Platforms using several cores with different performance characteristics make a challenge the selection of the best programming model, based on the corresponding executing algorithm. To make this study, there are approaches in the literature, that go from comparing in isolation the corresponding programming models' primitives to the evaluation of a complete set of benchmarks. Our study shows that none of them may provide enough information for a HPC application to make a programming model selection. In addition, modern platforms are modifying the memory hierarchy, evolving to larger shared and private caches or NUMA regions making the memory wall an issue to consider depending on the memory access patterns of applications. In this work, we propose a methodology based on Parallel Programming Patterns to consider intra and inter socket communication. In this sense, we analyze MPI, OpenMP and the hybrid solution MPI/OpenMP in shared-memory environments. We demonstrate that the proposed comparison methodology may give more accurate predictions in performance for given HPC applications and consequently a useful tool to select the appropriate parallel programming model.

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Hierarchical Clustering of Spatial Urban Data

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Keywords. Machine Learning; Urban Data; Clustering.

The growth in data gathered in urban contexts opens up to their exploitation for improving citizen quality-of-life and city management issues, like resource planning (water, electricity), traffic, air and water quality, public policy and public safety services. Moreover, most of the available data are geo-referenced, due to the large-scale diffusion of GPS and scanning devices[2]. Considering such an abundance of data, a very desirable and common task is to identify homogeneous regions in spatial data by partitioning a city into uniform regions based on pollution density, mobility spikes, crimes, or on other characteristics[3]. Density-based clustering algorithms have been shown to be very suitable to detect density-based regions, i.e. areas in which urban events occur with higher density than the remainder of the dataset. Nevertheless, an important issue of such algorithms is that, due to the adoption of global parameters, they fail to identify clusters with varied densities, unless the clusters are clearly separated by sparse regions[1]. In this paper we provide a preliminary analysis about how hierarchical clustering can be used to discover spatial clusters of different densities, in spatial urban data. The algorithm can automatically estimate the area of the data having different densities, it can automatically estimate parameters for each cluster so as to reduce the requirement for human intervention or domain knowledge.

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Numerical Analysis of Complex and Multiscale Systems

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Numerical Algorithms for the Parametric Continuation of Stiff ODEs deriving from the Modeling of Combustion with Detailed Chemical Mechanisms

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Keywords. Bifurcation and stability of dynamical systems; Parametric continuation; Numerical algorithms; Computational efficiency.

The use of detailed chemical mechanisms is becoming increasingly necessary during the actual transition of the energy production from fossil to renewable fuels. Indeed, the modern renewable fuels are characterized by a composition more complex than traditional fossil fuels due to the variability of the properties of the primary source, i.e. biomass. Parametric continuation can be a formidable tool to study the behavior of these new fuels allowing to promptly assess equilibrium conditions varying the main operative parameters. However, parametric continuation is a very computationally demanding procedure, both for the number of elementary operations needed and for the memory requirements. Actually, only very recently some approaches that allow to afford this computation with chemical mechanisms composed of hundreds of chemical species and thousands of reaction have been proposed [1–3].

Starting from the procedure illustrated in [2], this paper illustrates further improvements of key steps that usually represents a bottleneck for the effective computation of parametric continuations and for the identification of bifurcation points.

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Modelling and Analysis of Functional Connectivity in EEG source level in Chlidren with Epilepsy

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Keywords. Source Localization; Reconstruction of Functional Connectivity; Epilepsy.

Epilepsy affects more than 65 million people worldwide and around 10.5 million of them are children. Although many children self-heal before adulthood, it has been shown that children with epilepsy confront various problems in learning, attention as well as in memory capacity. Thus, the systematic study of the brain (dys)functionality, and ultimately the design of proper treatments is one of the most challenging problems in neuroscience. Towards this aim, neuroimaging techniques and in particular EEG recordings, most commonly used for clinical assessment play an important role. However, an analysis at the scalp level does not give insight to the functionality and interactions of the “true” brain regions. On the other hand, the inverse problem, i.e. that of identifying the involved brain regions from scalp recordings is an ill-defined problem and as such a comparison between various numerical methods that solve it is critical. Here, we reconstruct the functional connectivity of brain activity of children with epilepsy based on EEG recordings of one-back matching visual discrimination working memory task [1, 2]. We first solve the inverse source localisation problem by using three methods, namely the standarized Low Resolution Electromagnetic Tomography (sLORETA), the weighted Minimum Norm Estimation (wMNE), and the dynamic Statistical Parametric Mapping (dSPM). Then using both linear and nonlinear causality models we reconstruct the functional connectivity network between the sources. A comparative analysis between methods and groups (epileptic vs. children) reveals different spatio-temporal patterns that may serve as “biomarkers” for diagnostic purposes and ultimately localised treatment.

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Pattern formation and numerical bifurcation analysis for a vegetation model

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Keywords. PDE; vegetation dynamics; Turing pattern.

Several mathematical models were formulated as systems of PDEs to simulate vegetation patterns. These vegetation patterns are observed in numerous regions around the world ([1]) and it has been hypothesized that their development is affected by global phenomena like climate change ([1]).
These mathematical models that has been used to simulate the vegetation pattern formation consider positive feedback mechanisms between water and biomass. Moreover, some studies explain pattern formation as a consequence of negative plant-soil feedback interactions.
In this work we present a pattern formation and a numerical bifurcation analysis of a vegetation model which includes negative plant-soil feedback, based on the PDE model of [3]. The study has revealed the existence of variety of different spatial patterns in the space arising from Turing bifurcation of the homogeneous state. The effect of the precipitation rate is analyzed as system parameter. Coexistence between different patterns has been observed in a wide range of precipitation rate. Moreover the effect of boundary conditions on the nonlinear dynamics is also discussed.

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The dynamics of a ring network with switched connections

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Keywords. Ring Network; Periodically Forced Systems; Bifurcation Analysis.

In this work we analyse transitions between symmetric and asymmetric regimes in a ring network with periodically forced connections [1–3]. In particular, the network consists of a ring where the connections are periodically switched (ON/OFF) with a circular law. We consider, as an example, a sequence of n reactors where the feed position is periodically shifted according to a permutation law. We analyse the symmetry-breaking phenomena which are consequence of interaction between the natural and external forcing action. As the main parameters are varied due to the presence of Neimark-Saicker bifurcations, the system exhibits periodic regimes where the periods are exact multiples of the period of the forcing or quasi-periodic regimes. In addition to the standard phenomenon of frequency locking, we observe symmetry breaking transitions. While in a symmetric regime all the reactors in the network have the same time history, symmetry breaking is always coupled to a situation in which one or more reactors of the ring exhibit a greater temperature than the others. We found that symmetry is broken when the rotational number of the limit cycle, which arises from the Neimark-Saicker bifurcation, is an specific ratio. Finally, symmetry locking and resonance regions are computed through the bifurcational analysis to detect the critical parameters which mark the symmetry-breaking transitions.

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Numerical approximation of center, stable and unstable manifolds of multiscale/stochastic systems

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Keywords. Multiscale/ Stochastic Systems; Numerical Approximation of Manifolds; Equation-Free approach.

The numerical approximation of center, unstable and stable ivariant manifolds is important for a series of system-level tasks, particularly for the analysis and control large-scale systems. For example, embedding the high-dimensional dynamics on the center manifold allows the stability analysis and the control on a lower dimensional space. Here, we extend our previous work [1] to address a numerical methodology for the computation of such manifolds for multiscale/stochastic systems for which a "good" macroscopic description in the form of Ordinary (ODEs) and/or Partial Differential Equations (PDEs) does not explicitly/ analytically exists in a closed form. Thus, the assumption is that we have a detailed dynamical simulator of a complex system in the form of Monte-Carlo, Brownian dynamics, Agent-based e.t.c. but we don't have a explicitly a system of ODEs or PDEs in a closed form for the "slow" evolving variables. Based on this assumption, Gear & Kevrekidis [2] and Gear et al. [3] addressed an approach to compute "slow" manifolds by restricting the higher-order derivatives of the "fast" variables to zero. Our numerical scheme is a three-tier one including the (a) on "demand" detection of the (coarse-grained) non-hyperbolic equilibrium, (b) stability analysis of the critical point(s), and (c) approximation of local invariant manifolds by identifying the nuemrical quantities required (residuals, Jacobians, Hessians, etc)

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Effect of human interaction on forest-grassland dynamics: a numerical bifurcation analysis

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Keywords. Numerical Bifurcation Analysis; Ecosystems; Human Interaction.

Many ecosytems are characterized by multistability and/or oscillating regimes. Sudden shifts between states may emerge due to external disturbances and/or human intervention. Thus understanding how disturbances and human interaction influence the dynamics of ecosystems is very important for the prevention and control of ecological catastrophic shifts which may manifest as "sudden" phase transitions towards undesirable states [1, 2]. Examples of such ecosystems are the forest-grassland mosaic ecosystems [3]. Thus, human preference and consequent actions have a direct effect on these transitions. Thus, understanding how the stability of such systems is affected by external perturbations and human intervention is of primary importance for their management and urban design. In this work we perform a one and two parameter numerical bifurcation analysis of a forest-grassland ecosystem model proposed by [3] which includes human inference. Our numerical analysis reveals that this simple model is able to approximate complex nonlinear behaviour including multistability and oscillations with shifts characterized by both catastrophic and smooth transitions including Bautin bifurcations [4].

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Variational Analysis and Optimization Methods with Applications in Finance and Economics

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Dynamic Risk Aversion and Risk Vulnerability

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Keywords. Dynamic risk; Vulnerability; Portfolio problem.

This talk deals with money utility functions, in which money values are allowed from an arbitrary nonempty closed subset of real numbers, and therefore considers the classical case, in which this subset is the set of all real numbers, as well as the discrete case, in which this subset is the set of all integer numbers. The latter case has not yet received attention in literature, even though it may be seen as more appropriate than the continuous case for application in the real world. Risk aversion and risk premium are discussed and an analogue of Pratt's fundamental theorem is proved, while temperance, prudence and risk vulnerability are also scrutinized. Applications such as the standard portfolio problem are examined and multiple examples with varying underlying money set options are illustrated. This theme brings together the fields of mathematics (dynamic equations on time scales, see [2]) and economics (the economics of risk and time, see [3]). New results and example will be presented.

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Characterization of efficient solutions in nonsmooth multiobjective problems using generalized invexity

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Keywords. Optimality conditions; Multiobjective optimization; Constraint qualificatrion; Semi-infinite optimization.

A multiobjective semi-infinite programming (MOSIP in brief) is an optimization problem where two or more objectives are to be minimized on a set of feasible solutions described by infinitely many inequality constraint functions. The purpose of characterizing the efficient solutions of MOSIP is to provide the necessary and sufficient conditions for its optimal points. This characterization has been studied by many authors in smooth and nonsmooth cases. In all the articles in this field, the necessary conditions in Fritz-John (FJ) type are presented under some special continuity assumption respect to index set of constraints, the necessary conditions in Karush-Kahn-Tucker (KKT) type is stared under satisfying some constraint qualifications, and the sufficient conditions in FJ and KKT types are organized under convexity, quasiconvexity\pseudoconvexity, and invexity assumptions for objective and restriction functions. In the present paper, we prove the FJ necessary condition under an assumption, named PLV property, which is weaker that continuity assumption. Then, we justify the KKT necessary condition under a weak constrain qualification that is defined under an special kind of generalized invexity, called $(\mathit{\Phi}, \rho)-$invexity. Finally, we show that the FJ and KKT sufficient conditions are valid under $(\mathit{\Phi}, \rho)-$invexity.

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Discrete Models for Dynamic Competitive Economic Equilibrium Problems

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Keywords. Economic equilibrium problem; Discrete equilibrium problem.

Equilibrium is a central concept in numerous disciplines including economics, management science, operations research, and engineering. We consider a discrete dynamic competitive economic equilibrium problem in terms of maximization of utility functions and of excess demand functions. We study the discrete equilibrium problem by means of a discrete time-dependent quasivariational inequality in the discrete space $l^2([0,T]_Z, R)$. We ensure an existence result of discrete time-dependent equilibrium solutions.

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Qualifications and stationary conditions for nonsmooth multiobjective mathematical programming problem with vanishing constraints

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Keywords. Stationary conditions; MPVC; Constraint qualification.

In the context of optimization theory, the concept of multiobjective programming is very popular. At the other hand, a difficult class of optimization problems, introduced in 2007 and called mathematical programming with vanishing constraints (MPVC, in brief), has attracted the attention of researchers, due to their theoretical and practical scope. From the combination of these two issues, we will find a new important problem that we call it multiobjective mathematical programming problem with vanishing constraints (MMPVC). Defining of constraint qualifications and presenting of optimality conditions (named, stationary conditions) are two important features in studying of MPVCs, and the smoothness of considered functions are assumed in almost all these articles. The goal of present paper is extension of these results to the MMPVCs with nonsmooth objective and constraint functions. For this end, we introduce several kinds of constraint qualifications for nonsmooth MMPVCs and we study the relationships between them. Then, we apply the constraint qualifications in finding of necessary stationary conditions. Finally, we show these stationary conditions are sufficient for optimality (efficiently), too.

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Agent-based models of spatial aggregation and their continuum limits

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Keywords. agent-based models, bacterial aggregation, wealth hot-spots

Agent-based models are widely used in numerous applications. They have an advantage of being easy to formulate and to implement on a computer. On the other hand, to get any mathematical insight (motivated by, but going beyond computer simulations) often requires looking at the continuum limit where the number of agents becomes large. In this talk I give several examples of agent- based models, starting from their derivation to taking their continuum limit, to analysis of the resulting continuum equations.

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A model of optimal consumption and borrowing with random time scale

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Keywords. time scale; optimal control; funactional Newton method.

This work is dedicated to modelling economic dynamics with random time scale. The need for such model appears when a theoretical model formulated in continuous time is applied to numerical computations using the statistical data is discrete time. Observed data have certain characteristic period - hour, month, quarter, year, whereas the underlying economic processes, especially in what relates to financial transactions, inventory management and trade in durable goods, may not have periodicity at all, or have a characteristic time of change different from what is observed on the available time. For example, for financial accounts with equal balances at the end of period, the turnover during the period might differ tenfold.

We propose a solution in the form a continuous time model where interactions of agents interactions of agents are random exchanges of finite portions of products and money at random points in time. In this framework, the economic agent determines the volume, but not the moments of the transactions and their order. The paper presents a correct formal description of optimal consumption and borrowing as a stochastic optimal control problem, which we study using the optimality conditions in the Lagrange's form. The solution appears to have a boundary layer near the end of planning horizon where the optimal control satisfies the specific functional equation. This equation was studied numerically using the functional Newton method [1] adapted for a two-dimensional case.

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Philosophy of Mathematics: Applicability, Practice, and Numerical Computations

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On the notion of mathematical formalism

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Keywords. mathematical formalism; models; scientific practice.

This paper is about how scientists retrieve information from their mathematical models. Whereas the *representational* elements of models have been analyzed by several philosophy of science, their capacity to allow for predictions and explanations requires further investigation. The main proposal here is that a new component has to be taken into philosophical account, namely, mathematical formalism. A mathematical formalism is a mathematical theory *as it is used by empirical scientists*, especially physicists, who want to draw inferences from their models. Mathematical formalisms are thus both constrained by the logical relationships among mathematical theories and by the historical development of physics and the way physicists calculate the (usually) approximate solutions of their models. The life of mathematical formalisms is thus partly determined by practices that develop outside the realm of mathematics. The paper will examine several examples of formalisms in order to bring their components into light: calculus, cellular automata, Fourier transforms, and others.

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A new syntax for diagrammatic logic: a generic figures approach

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Keywords. Existential Graphs, Categorical Logic, Generic Figures

In this paper we present a new syntactical representation of the, often overlooked, diagrammatic models for propositional and predicate logic introduced by C.S. Peirce towards the end of the 19th century (so called Alpha and Beta Existential graphs). These are representations of syntax and semantic for propositional and first-order logic solely based on very simple diagrams and the topological/combinatorial relations that such diagrams entail.

For too long these graphs have been considered just a curious variation of standard linear notation. The renewed interest in diagrammatic reasoning via Category Theory however (see the work in diagrammatic quantum computation done by Bob Coecke [1], Spivak's wiring diagrams [4] and Ahti Pietarinen's diagrammatic proof analysis [2]) has motivated us to take a closer look to the inner structure of Peirce's graphs via the categorical notion of *generic figure* developed by Gonzalo Reyes [3].

The notion that category theory is a powerful and efficient framework for models of logic is based on the idea that objects in a suitable category model proposition, whereas morphisms model proofs. In our work we take a different approach, as we model propositions as functors from a suitable "base" category into the category of sets. Therefore, some of the lurking problems that arise when trying to formalize in a rigorous setting Peirce's diagrams, are solved in a single stroke by presenting the very simple base category that "generates" the desired language. In some sense, ours is a hybrid model that aims to fill an intellectual void in the link between the categorical and the classical approach to logic.

In this paper we provide the basic categorical background needed to define our base categories and present a full account of what these categories look like.

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Concepts of approximate solutions and the finite element method

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Keywords. Computer simulation; Numerical solution; Finite element; Variational crime

This paper discusses epistemologically unique difficulties associated with the solution of mathematical problems by means of the finite element method. This method, used to obtain approximate solutions to multidimensional systems with possibly irregular boundary conditions, has received comparatively little attention in the philosophical literature, despite being the most dependable computational method used by structural engineers and other modelers handling complex real-world systems. As most numerical methods that are part of the standard numerical analysis curriculum do, this method breaks from the classical perspective on exact mathematical solutions, as it involves error-control strategies within given modeling contexts. This transition requires criteria to assess the justification of solutions that contain more complex semantic elements, whose murkier underlying logic is essential to a philosophical understanding of the lessons of applied mathematics.

To be sure, among practitioners, there is a practical acceptance of the finite element method as a method to overcome the inferential opacity of the models they use, mainly because it has proved to be tremendously successful. However, the finite element method differs in important respects from other numerical methods. What makes the method so advantageous in practice is its discretization scheme, which is applicable to objects of any shape and dimension. Officially, each simplified inside element is locally analyzed, and then they are recursively "glued" to obtain the solution over the whole domain. However, this presents applied mathematicians with a dilemma, since the standard mathematically sound methodology to perform local-global "gluing" is typically computationally intractable in this situation. Perhaps surprisingly, computational expediency is typically chosen over mathematical soundness. Strang has characterized this methodological gambit as a "variational crime." I explain how committing variational crimes is a paradigmatic violation of epistemological principles that are typically used to make sense of approximation in applied mathematics. On that basis, I argue that the epistemological meaning of these innovations and difficulties in the justification of the relationship between the system and the solution lies in an enriched concept of validity of solutions that is in line with recently developed methods of a posteriori error analysis.

A comparison of new approaches to infinity

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Keywords. Infinite; Infinitesimal; Nonstandard.

Since Georg Cantor introduced infinite numbers, in the Eighties of the Nineteenth century, and "proved" that infinitesimals were inconsistent, the study of the latter continued in occasional ways in the realm of Non-archimedean fields (Veronese, Levi-Civita, Hardy). Only in 1963 Abraham Robinson was able, doting on logical concepts, to show that analysis and other mathematical disciplines could be developed in a systematic way by infinitesimal methods which he named "non-standard". He showed their power and relative consistency, vindicating Leibniz's ideas of (roughly) elementary conservative extensions.

The non-standard methods have proved their efficacy in many mathematical disciplines. Recently, after their success, new approaches to the concept of infinity have been independently devised by Vieri Benci (in Pisa, IT) and by Yaroslav Sergeyev (in Cosenza, IT) – besides others less systematic (such as that of Detlef Laugwitz).

Both Benci and Sergeyev start from the recovery of Euclid's fifth common notion – "the whole is greater than the parts" – which is violated by Cantor's definition of sameness of cardinality through the existence of a bijection. Benci has tried to build a theory of a different concept of cardinality, named numerosity, using the non-standard frame and concepts. Sergeyev is more interested in the computational aspects of his Grossone, the number of the natural numbers.

Actually the two approaches stem from two very different conceptions of mathematics and of mathematical research, which we will discuss and try to elucidate.

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Re-evaluating the role of mathematics in biology: Is systems biology a break with the past?

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In "Untimely Births of a Mathematical Biology", Fox Keller (2003) analyzes the reasons behind the historical rejection by experimental biologists of mathematical methods and models in their own practices. One of the foremost reasons for this rejection according Fox Keller was the fact that mathematical models of biological phenomena were heavily idealized. Idealization and simplification were nonetheless advocated for in population ecology by Levins in 1966 on philosophical grounds and much of the mathematical modeling in fields studying biology seem to have stuck to this stricture, despite the opposition of biologists. While traditional mathematical biological fields like biophysics and mathematical ecology have persisted and developed, the advent of modern systems biology around the year 2000 arguably represents something of change to the traditional emphasis on idealized modeling. Systems biologists, often engineers, aim to some extent to reproduce the complexity of a biological system within a computational model, on the basis that only by doing so can we really make reliable predictions about the behavior of such systems in response to perturbations, and achieve forms of understanding (about robustness for instance) unobtainable through idealization alone. In this paper we evaluate whether or not the advent of modern systems biology can be said to transform the historical relationship between mathematics and biology, and in effect whether it is transforming the attitudes of biologists by conceding the limited value of highly idealized models in the face of complexity and variability. We will argue that while modern systems biology is a departure from highly idealized modeling in some respects, the sheer complexity of biological systems necessitates significant forms of abstraction regardless, which still complicates the relationships between experimental biologists and modelers. There are good grounds to support biologists' intuitions about the limits on the power of mathematical models to accurately represent biological systems. In practice these factors do oblige systems biologists to rely on simplified and abstract models, and pursue goals other than detailed representation alone. This does not however mean a return to idealization. Many novel uses of models have arisen as a result which often strike experimental biologists as reasonable, and may indeed represent a genuine break with the use of mathematics in past biology.

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Applied Infinity: Accuracy and Artefact

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Keywords. Grossone; numerosity; arbitrariness; infinity; cardinality; accuracy; artefacts.

Recently, theories of infinite quantity alternative to Cantor's have emerged. We will consider the theories of numerosity and grossone. Both are Euclidean theories in the sense that they satisfy the principle that a set has more elements than any of its proper subsets. In [3], we argued that any Euclidean theory of set size suffers from arbitrariness. However, proponents of numerosity and grossone adopt epistemic and methodological stances that may be taken to defuse concerns about arbitrariness. Here we investigate the extent to which such stances do defuse practical concerns about arbitrariness in applications. We first consider numerosity theory from [1] and its application to probability in [1], where numerosity itself is defended against the charge of arbitrariness through a skeptical and pragmatic stance, arguing that probability models can only track chance in a mediated way. However, this claim does not diminish the concern that some models can mislead us more than others. The controversial theory of grossone emphasises the finitude of human capacities and the distinction between numbers and the linguistic tools used to represent them [4]. An analogy is drawn between numeral systems and optical instruments: observations with differently powered lenses differ in accuracy but are not simply incorrect; results about quantity are always relative to the numeral system used. However, the notion of accuracy suggests that there is an ultimate truth that the more accurate instruments better reveal, and it is not clear that this is the case for all of the free choices involved in constructing a theory of grossone. On the other hand, the applications of grossone may not depend on the arbitrary features of the theory.

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Bijections and Euclidean set-size measures

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Keywords. Euclidean set-size; numerical infinities; invariance.

In recent years, the general project of introducing measures for infinite collections (notably $\mathbb{N}$ and its infinite parts) that discriminate between whole and part has been met by some penetrating criticism questioning the serviceability of such measures in light of distinctive limitations. In particular, [1] showed that whole-part discriminations in a discrete distribution over $\mathbb{N}$ violate the property that a relabelling of a sequence should not affect its probability. Even more significantly, [3] showed that, in elementary metric spaces, translations and rotations may affect the Euclidean measures of sequences. It is as if shifting around a given collection should modify the way its items are counted. In this talk I investigate these results in a constructive spirit, showing in what way they can be regarded as pointers to a key *desideratum* that a fruitful approach to Euclidean measures of infinite collections should take. In particular, I focus on the fact that the failures of invariance pointed out by [1, 3] are not caused solely by the requirement that measures should be Euclidean, but also by the presuppositions that classical bijections (i.e. ones identifying, relative to size, any two sequences) are an acceptable instrumentality for size comparisons. It is in fact the interaction of Euclidean measures and classical bijections that gives rise to the striking invariance failures detected in the literature. A promising way to avoid them is to devise a refinement in the treatment of bijections, along the lines suggested by [4], in such a way that whole and part are linked by refined bijections. I discuss the way in which a specific, formal notion of refinement can be used to circumvent the issues pointed out in [1, 3] with reference to the axiomatic framework developed in [2].

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Affinity of views of Florenskij and Sergeyev on numeral systems and their applications in mathematics and computer science

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Keywords. Numeral systems; numbers and numerals; Infinity Computer.

In 1916 in the work *Reduction of numbers*, P.A. Florenskij studied properties of numbers written down in a numeral system with a base α. His discoveries can be briefly summarized as follows: 1) all numbers have a geometric interpretation and some numbers, for a specific value of α, can be represented by points (indecomposable numbers in a geometrical sense) and the others can be represented by polygons (decomposable numbers in this geometrical sense); 2) there are no indecomposable numbers, to show this it is sufficient to increase the base of the numeral system α; in other words, by increasing α one can see certain features that cannot be previously observed; 3) modification of a numeral system changes observed properties of numbers.

It seems that these interesting ideas regarding the influence of numeral systems on visible properties of numbers have not been in demand for a long time. However, in the beginning of the XXIth century, a new methodology using a fresh numeral system with an infinite base has been proposed (see [1]). This methodology emphasizes the crucial importance of numeral systems with respect to observability of numbers. It has allowed people to obtain a series of important results in a variety of applied and theoretical research areas (see [1]) and has attracted an attention of philosophers of mathematics (see [2-4]).

In this talk, we discuss both points of view and emphasize their importance for modern applied mathematics and computer science.

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Applied versus Situated Mathematics in Ancient Egypt: Bridging the Gap between Theory and Practice

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Keywords. Situated mathematics; Ancient Egypt; Hellenocentrism.

This historiographical study aims at introducing the category of "situated mathematics" to the case of Ancient Egypt. However, unlike Situated Learning Theory (Lave, 1988; Greeno, Moore & Smith, 1993), which is based on ethnographic relativity, in this paper, the goal is to analyse a mathematical craft knowledge based on concrete particulars and case studies, which is ubiquitous in all human activity, and which even covers, as a specific case, the Hellenistic style, where theoretical constructs do not stand apart from practice, but instead remain grounded in it. On the one hand, the dominant Hellenocentric approach seeks to generate a body of principles that could then be applied in other fields, as $M_A : T \to P$, where $T =$ theory and $P =$ practice/applications, in accordance with Platonist arguments (Plato, *Rep.*, VII, 527b). This practice of translating theoretical tenets directly into specific applications needs to be challenged. On the other hand, in situated mathematics, more complex transfer relations can be given like those of the type $M_S : (T \leftrightarrow P) \vee \left(P \to \{P'_i\}_{i\in I}\right)$, with $P'_i =$ other specific practices, rather than focusing in the production of supposedly context- free principles, that are independent of the contingencies of particular cases. Therefore, the concept of applied mathematics would be included within that of situated mathematics, and it would be a concrete case of it. The differences would then lie on the knowledge, skills and techniques of the specific original context, therefore contributing in other working areas.

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In Quest for Invariant Structures through Graph Theory, Groups and Mechanics: Methodological Aspects in the History of Applied Mathematics

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Keywords. Invariants; graph theory; geometry.

The purpose of this paper is to analyse a geometrical case study as a sample of an intended methodology based on invariant theory's strategies, which have been developed particularly throughout the nineteenth century as one of the cornerstones of mathematics (Rota, 1998: 41), and whose resolution was reached by means of a combination of different disciplines: graph theory, mechanics and group theory, among others.

This case study presents the "perfect squared rectangle problem", that is an exhaustive classification of the dissection of a rectangle into a finite number of unequal squares. Despite its simplicity, in both description and mathematical resolution, it provides plausible elements of generalization from"the 'applied field' of mathematics" (Epple, Kjeldsen & Siegmund-Schultze, 2013: 658), as a special case of applied mathematical toolkit (Archibald, 2013: 715), related to the practice of invariant strategies that remain fixed through changes.

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Regular Presentations

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Rational Approximations of the Fractional Laplacian in Reaction-Diffusion Problems

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Keywords. Fractional Laplacian; matrix functions; Gauss-Jacobi rule; Padé approximants.

In this talk we consider mathematical models of fractional order in space in which the integer-order differential operator is replaced by a fractional correspondent. Such models have become increasingly used because they provide an adequate description of many processes that present an anomalous diffusion. In particular, we focus on the numerical solution of fractional in space reaction-diffusion equations on bounded domains under homogeneous Dirichlet boundary conditions. By using the so-called *matrix transfer technique* introduced by Ilić et al. in [3, 4], the fractional Laplacian is replaced by a matrix which is generally dense. The proposed approach is based on the approximation of this matrix through the product of two appropriate banded matrices [1, 2]. This leads to a semi-linear initial value problem in which the involved matrices are sparse. The numerical experiments we present confirm the effectiveness of the proposed approach.

Acknowledgements.

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Stability of DESA Optimization Algorithm and its Application to time series Susceptible-Infected-Recovered models

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Keywords. Differential evolution - simulated annealing; time series SIR; influenza-like fever.

Optimization of mathematical models derived from statistical inference techniques allows us to combine infectious disease theory and empirical data, unraveling the difficulty of predicting future trends from chaotic time series realizations. However, optimizing the parameters of a continuous-time process Susceptible-Infected-Recovered (SIR) model against the one state variable time-series data is a challenging mathematical problem.

This study investigates the dynamics of the hybrid evolutionary optimization algorithm, Differential Evolution-Simulated Annealing (DESA) algorithm with DE/rand/1/bin and SA-like selection operators. The stability of the DESA-population is established using Lyapunov?s stability theorems. Numerical experiments in the least squares fitting of chaotic time series processes show that DESA algorithm obtained global parameter estimates.

Specifically, DESA algorithm is used to optimize the parameters of the time-series SIR model for the weekly reported incidence of influenza-like fever in Baguio City, Philippines.

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Applying Linear Optimization Methods to Problems with Internal Dependencies

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Keywords. Linear Optimization; Network Planing; Parametric Programming.

There are many problems that could be presented as linear optimization problems if you discard some interconnections between variables. For example, we can have a normal set of inequalities that can be solved by methods of linear programming. But additionally, we can have a set of requirements that we can not easily convert to inequalities.

If so, we can not use traditional linear programming methods such as Simplex method, since they are defined on sets of inequalities. A method to find at least a good approximation of the optimal result was proposed in [1]. The main idea of this method is to split the problem into smaller ones where there are no special requirements present. Solving these sub-problems should be possible by means of any applicable linear programming method. Possible restrictions can be then applied manually.

In this way, all specific restrictions could be satisfied and all problems solved before will have their impact on those solved subsequently. But an influence in reverse direction is still missing. Sub-problems solved later can not influence sub-problems that were solved previously, even if they were connected.

A way to fix this issue is proposed in this presentation (see also [2]). We can make a guess about future values of variables moved to sub-problems that will be solved later and use them instead of actual values. A genetic algorithm could be used on those predicted values to minimize the error.

The method was tested for an automated creation of syllabus in educational institutions and was implemented in the software Study Plan Generator now in use at the Technical College of the Dniprovsk State Technical University.

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Preserving Stone Fruits

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Keywords. Prolate Spheroid; Heat Conduction; Stone Fruits.

Rapid cooling of stone fruits is common and necessary for extending the shelf life of such products. While several studies have been conducted to estimate the cooling time, it has usually been the case that such fruits (olives, dates, etc.) are modelled as spheres with internal spherical cores. The motive for such simplification is that the governing heat differential equation is easily solved in spherical coordinates. It is obvious that such fruits are not spherical. They are in the shape of prolate spheroids (i. e. elongated spheres with different major and minor axes). Such simplifications in the geometry of these fruits, naturally, induce errors in the estimation of the time needed and consequently in the amount of energy used in the cooling process.

In this research, we accurately determine the cooling time of stone fruits using their natural prolate spheroidal shapes. To solve the heat conduction over a prolate spheroid, we use a specially fit coordinates system, namely the prolate spheroidal coordinates system. Unlike the well-known coordinates systems (rectangular, cylindrical, and spherical), this system is capable of appropriately hosting such geometry. We consider different cooling conditions through varying the Biot number which is a dimensionless number that combines the effects of the conduction properties of the stone fruits, and the convection strength of the cooling media.

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Conditions of the Stability Preservation under Discretization of a Class of Nonlinear Time-Delay Systems

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Keywords. Nonlinear system, discretization; stability; convergence rate.

Preserving qualitative characteristics, when passing from differential equations to difference ones, is a fundamental and challenging research problem [1]. In many cases it is necessary to modify numerical schemes in order to preserve required characteristics. Such modifications result in conservative numerical schemes [2]. However, the use of conservative schemes significantly complicates corresponding difference systems. Therefore, from a practical point of view, it is important to determine classes of systems for which discretization preserves qualitative properties without modifications of computational schemes.

In this contribution, nonlinear differential systems with nonlinearities satisfying sector constraints and with constant delays are studied. Such systems belong to well-known class of Persidskii-type systems, and they are widely used for modeling automatic control systems and neural networks, see [3]. We derive conditions of the stability preservation under discretization of the considered differential systems. The fulfilment of these conditions guarantees that the zero solutions of the corresponding difference systems are asymptotically stable for arbitrary values of delays. Moreover, estimates of the convergence rate of solutions are obtained.

The proposed approaches are used for the stability analysis of a discrete-time model of population dynamics.

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A matlab code for the numerical solution of Multiparameter Spectral Problems

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Keywords. Multiparameter spectral problems; Finite differences.

Many applications in physics and chemistry are connected with Sturm Liouville problems. For this reason, the numerical solution of such problems has been widely investigated in the recent years. Multiparameter spectral problems may be considered as a generalization of such problems, even if their solution requires additional care, since the discretized problem cannot be solved by standard algebraic techniques.

The goal of this talk is to present a new matlab code for the solution of multiparameter spectral problems for ordinary differential equations. The code is able to compute the couple eigen-parameters / eigen-functions corresponding to specified number of oscillations. It is based on High Order Finite Difference Schemes [1] that allow to obtain a discrete multi-parameter nonlinear system of equations.

Due to the intrinsic difficulty, the problem is solved in two different stages. The first one is necessary to get an initial estimation of the eigen-parameters and of the eigen-functions using constant stepsize; the second stage has the purpose of computing an accurate approximation of both eigen-parameters and eigen-functions applying a variable stepsize and a variable order.

The code will be tested on several problems, in particular arising from the solution of the so-called 'whispering gallery' modes (WGMs) occurring inside a prolate and oblate spheroidal cavity [2,3].

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A Reinforcement Learning Approach to a Multi-agent N-armed Functional Bandit

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Keywords. multi-armed bandit; N-armed bandit; reinforcement learning; congestion games.

The classic N-armed bandit problem [1] is widely used as an example in the area of reinforcement learning to demonstrate the requirement for an agent to balance its strategy between exploration and exploitation. One can view this as a one state Markov Decision Process, with the agent returning back to the start state after receiving the reward for the chosen action. Many variants of this problem, such as the binary, Bernoulli and restless N-armed bandit machine, have been studied and practical applications include adaptive routing, portfolio design and clinical trials.

In this study we consider three extensions to this problem, the first is to consider rewards which are dependent on a sequence of k lever pulls, *i.e.*, an episode of the game. The objective of the agent is to generate a policy that maximises the expected reward of playing an episode of the game.

Second, multiple agents simultaneously play the bandit machine receiving rewards that are dependent on the actions of other agents, *e.g.*, the payoff matrix of a sequential social dilemma given in examples such as the Prisoner's Dilemma. Game theory concepts, such as greed and fear, are interrogated to understand an agent's motivation for co-operation, using a deep centralised and decentralised approach [2].

Finally we present a multi-agent functional variant that can be applied to network congestion games [3] such as the classic Traffic Assignment Problem [TAP] and explore the effectiveness and applicability of our reinforcement learning approach with known approaches such as Frank-Wolfe, Bar-Gera and Dial [4].

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Algorithms of 3D wind field reconstructing by lidar remote sensing data

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Keywords. Remote sensing; wind lidar; wind field recovery.

Data on the spatial distribution of the wind parameters in the surface layer is an important factor for aviation. To obtain this data, Doppler wind lidars scanning in PPI (Plan Position Indicator) mode with low elevation angles are used. However, only the wind component along the measurement direction is directly measured, and post-processing methods are required to determine wind speed and direction. Many works deal with the problem of wind profile reconstructing by lidar data. However, the procedures for reconstructing wind parameters for PPI mode with low elevation angles are studied in less detail. In this case, the problem of wind field reconstruction is different, as to determine the wind vector, data from scanning in a small sector only can be used. This is due to the fact that the surface wind is characterized by time-space variability, and the wind field structure on a small scale is of most interest. For a good conditionality of the equations system for determining wind parameters, it is necessary to increase the size of the averaging region. On the other hand, smoothing of the wind field occurs when the residual error is calculated over a large area. In this paper, the performance of wind field reconstruction from lidar data is analysed. Algorithms of reconstruction using different versions of the least squares method are considered, as well as the use of data spikes filtering procedures. The weights were calculated inversely with the local approximation error. The data of real measurements obtained in various wind conditions were used as the initial data. The situations of a stationary wind field, a wind field with speed gusts, a wind field with fluctuations in direction, a wind field of variable speed and direction are considered. The questions of the use of regularization methods are considered. The influence of the averaging region on the quality of the reconstruction was analysed. Optimized dependences of the averaging area sizes as a function of the distance to the reconstruction point are obtained.

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Intelligent Management Systems in Hotels: Machine Learning Meets Optimization Heuristics

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Keywords. Machine learning and Intelligent optimization; Hotel revenue management; Simulation-Based Optimization; Optimization Heuristics.

The complexity of managing hotels to optimize quality and profits is growing. In addition to the traditional "property management" issues, activities related to revenue management (deciding what to sell, when to sell, to whom to sell, and for which price), to marketing and selling over multiple channels (e.g., Online Travel Agencies) are becoming of paramount importance to increase profitability. One witnesses a transition from "Property Management Systems" (PMS) to more global "Intelligent Management Systems" (IMS), which tend to be data-driven and based on flexible models and optimization.

In this context, hotel management is characterized by nonlinearities, many parameters and constraints, and stochasticity (in particular in the demand by customers). Effective heuristics can incorporate "learning" ("reactive" schemes) that update strategies based on the past history of the process (the history of the past reservations received up to a certain time) [1]. The most effective global optimization schemes [2] need to be combined with heuristics and massively parallel computation.

The experimental results show the effectiveness of intelligent heuristics with respect to exact optimization methods like dynamic programming, in particular for more constrained situations (cases when demand tends to saturate hotel room availability), when the simplifying assumptions needed to make the problem analytically treatable do not hold.

Acknowledgements.

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Novel pinning adaptive intermittent control for finite-time function projective synchronization of delayed nonlinear complex dynamical networks with hybrid coupling

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Keywords. finite-time function projective synchronization; nonlinear complex dynamical networks; pinning adaptive intermittent control, mixed time-varying delay, hybrid asymmetric coupling.

In this paper, finite-time function projective synchronization of delayed nonlinear complex dynamical networks (DNCDNs) with mixed time-varying and hybrid coupling delays is investigated via new pinning adaptive intermittent control method. The definition of finite-time function projective synchronization for DNCDNs is first studied. The designed controller ensures that the finite-time function projective synchronization of DNCDNs are proposed via new pinning adaptive intermittent control. Moreover, based on finite-time stability theory, a new differential inequality, Gronwall-Bellman inequality, common unitary matrix, Kronecker product of matrix, Wirtinger's inequality, improved Lyapunov–Krasovskii functional, new sufficient conditions for finite-time projective synchronization of DNCDNs are obtained and formulated in terms of linear matrix inequality. Furthermore, the minimum number of pinning nodes is determined by node dynamics required to achieve generalized finite-time function projective synchronization. Two examples based on Chua's circuit system and Lorenz chaotic system are included to illustrate the validity of the theoretical results.

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Verified solution of ODEs by Taylor models implemented in MATLAB/INTLAB

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Keywords. ordinary differential equations, Taylor models, INTLAB.

Taylor models have been used successfully for solving ordinary differential equations (ODEs) rigorously. Implementations are COSY INFINITY [1], ODEIntegretor [2], and RIOT [3]. Here, COSY INFINITY developed by Berz and Makino and their group is the most advanced implementation. Recently, we implemented the Taylor model approach in MATLAB/INTLAB [4].

We give a short introduction to Taylor models, their rigorous arithmetic, and the Taylor model method for enclosing solutions of ordinary differential equations in a verified manner. We only treat initial value problems

$$y' = f(t, y), \qquad y(t_0) = y_0$$

where the initial value y_0 may be an interval vector. For specific ODEs we demonstrate how to use and call our verified ODE solver. This is designed to be very similar to calling MATLAB's non-verified ODE solvers like ode45. Finally, results and run times are compared to those of COSY INFINITY, RIOT and Lohner's classical AWA.

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Bayesian Optimization of partially defined functions under unknown constraints: approximating feasible region boundary via Support Vector Machine

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Keywords. Bayesian Optimization; Constrained Global Optimization; Support Vector Machines.

We present a Bayesian Optimization (BO) [1] framework for optimizing a black-box, multi-extremal and expensive function, also partially defined [2], meaning that it cannot be computed outside the feasible region. Moreover, constraints defining the feasible region, within the search space, are unknown. The framework consists of two consecutive stages: a Support Vector Machine classifier approximates the boundary of the feasible region, then BO searches for a global feasible optimum. While in the first phase the next point to evaluate is chosen, over the entire search space, by dealing with the trade-off between improving the estimate of the boundary and discovering possible disconnected feasible regions, in the second phase BO is performed on the estimated feasibility region, only. We used 2D test functions to show how the framework works, then results on real-world simulation-optimization problems are reported. Indeed, simulation software often could be not able to compute function and/or constraints, due to computational reasons. Unlike previous works on BO with unknown constraints [3, 4], we do not rely on assumptions like a-priori knowledge on the number of constraints and their independence, since the classifier approximates the entire boundary of the feasible region, instead of having a model for each constraint.

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Dimensionality Reduction methods to scale Bayesian Optimization up

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Keywords. Bayesian Optimization; Dimensionality Reduction; Deep Autoencoders; Kernel.

Bayesian Optimization (BO) is a sample efficient method to optimize multi-extremal expensive black-box functions, under a given "budget", usually a limited number of function evaluations. Despite successful results in many application domains, especially Automatic Machine Learning, a well-known issue is that BO does not scale well with the number of dimensions. Random dropout was proposed [1], based on the assumption that just few dimensions are relevant for the BO process. Instead of a brute dropout, random embedding [2, 3] was suggested. This paper proposes to exploit the dimensionality reduction intrinsically offered by Deep autoencoders and then perform BO in the induced latent space. A first attempt to combine autoencoders and BO was presented in [4] to encode continuous representations of discrete variables and, eventually, reduce dimensionalty . We analyze the interplay between BO and the two mappings computed by the autoencoder - from the original to the latent space (encoding) and viceversa (deconding). To do not be stuck in local optima, we conclude that adaptive sampling in the original space is required when exploration is nullified by (inaccurate) decoding. Results on a set of examples with growing dimensionality are presented, along with a comparison with kernel methods, where encoding and decoding are replaced by kernel-pca and kernel, respectively.

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Pump Scheduling Optimization for water supply systems: a pilot in the peri-urban area of Milan

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Keywords. Pump Scheduling Optimization; Simulation-Optimization.

Pump Scheduling Optimization (PSO) is a challenging problem, with solutions proposed from both mathematical programming and machine learning communities [1]. Solving PSO consists to define which pumps are to be operated, and with which settings (e.g. speed), at different time of the day, with the goal to minimize energy costs. If there are storage tanks, cost reductions is performed by storing water when energy price is lower and then using this capacity during the remaining part of the day. Most of the approaches consider *explicit* pump scheduling, that is the state of each pump during predefined equal time intervals. This leads to a large number of decision variables (mixed-integer in the case that on/off and variable speed pumps coexist) [2]. Another approach considers, as decision variables, the start/end run times of the pumps [3], allowing to reduce the dimensionality of the problem and avoiding predefined equal time intervals. We present a PSO formalization, and preliminary results, for a case study whose pumps activation is currently decided depending on the pressure value monitored online. This policy aims at respecting lower and upper bounds on pressure, whose violation could lead to under-service and bursts, respectively. In our approach the goal is to also include energy costs minimization.

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Network Science Strategies for Accelerating the Training of Artificial Neural Networks

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Keywords. Network Science; Complex Networks; Artificial Neural Networks.

Deep Learning has relaunched artificial intelligence, opening it to an unprecedented number of new applications. A critical success factor is the ability to train deeper neural networks, striving for stable and accurate models. This translates into Artificial Neural Networks (ANN) that become unmanageable as the number of features increase.

While most current strategies focus on new machine learning algorithms, our approach is to employ network science strategies to tackle the complexity of the actual ANNs iteratively, that is at each epoch of the training process. The work presented herein originates in our earlier publications [1], [2], where we explored the acceleration effects obtained by enforcing, in turn, scale-freeness, small-worldness, and sparsity during the ANN training process. The efficiency of our approach has also been recently confirmed by independent researchers, who managed to train a million-node ANN on non-specialized laptops [3].

Encouraged by these results, we have now moved into looking at new network science strategies to pursue a further acceleration effect, whilst maintaining the accuracy and stability of the final models. Our method is independent from specific machine learning algorithms or datasets since we operate merely on the topology of the ANNs. We demonstrate various heuristics for orderly weight removal/replacement, which keep the ANN network sparse during the whole training without loss of efficiency. We also show how centrality metrics may be used to adjust the network sparsity during the training process.

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Numerical simulation of astrophysical and astrochemical problems on supercomputers

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Keywords. Astrophysics; high-performance computing; astrochemistry.

Implementation of a new vectorized high-order accuracy numerical method for solving gravitational gas dynamics equations on supercomputers equipped with Intel Xeon Skylake-SP or Intel Xeon Phi processors is presented in the paper. Combination of the Godunov method, the Harten-Lax-Van Leer method and the piecewise parabolic method on local stencil is at the basis of the method, that allows achieving high-order accuracy for smooth solutions and low dissipation on discontinuities. The impact of low-level code vectorization technique on performance is compared with compiler's auto-vectorization. Astrochemical model of formation and destruction of molecules based on chemical kinetics approach is presented. Numerical experiment results, which describe the mechanism of formation of O_2, CO, SiS, and SO, are shown.

Acknowledgements.

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An Efficient Solution to a Series of Weighted Least Squares Problems if Only Weights Vary

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Keywords. Weighted Least Squares; Fuzzy Logic; Interior Point Methods.

Solving a series of Weighted Linear Least Squares (WLLS) problems, when only the weights varies over time, is a problem frequently found in real world applications. To name a few, consider the problem of estimating the consequent parameters of a Takagi-Sugeno fuzzy system of the first order [1] or the problem of estimating the next approximating solution of a Linear Programming (LP) problem, when using Interior Point Methods (IPMs) [2], or the iterative re-weighted least squares problem. The problem is the following: given a real matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ (with $m \gg n$), a vector $\in \mathbb{R}^m$, and a series of weighting diagonal matrices $\mathbf{W}_i$, $\forall i = 1, ..., r$ (where $\mathbf{W}_i \in \mathbb{R}^{m \times m}$), find each vector $\mathbf{x}$ which minimizes the weighted 2-norm of $\mathbf{Ax} - \mathbf{b}$. In mathematical terms:

$$\min_{\mathbf{x}} \ \|\mathbf{Ax} - \mathbf{b}\|_{\mathbf{W}_i}.$$

The first idea that comes to mind to efficiently solve this series of problems where both $\mathbf{b}$ and (more importantly) $\mathbf{A}$ remain the same, is to figure out if one can factorize matrix $\mathbf{A}$ only once at the beginning, and reuse such factorization on all the r estimation problems. For instance, one could think about factorizing $\mathbf{A}$ using one of the standard factorizations, such as LU, QR, SVD or Cholesky. Unfortunately, this approach is very likely to not work. Even worse, proving this negative result is an even harder problem. The author spent a lot of time on trying to solve this puzzle, also asking their opinion to numerical linear algebra specialists. All of them were unanimous in considering the solution of each subsequent WLLS problem unrelated with that of the previous ones: at each step a new WLLS problem must be solved from scratch. In general we would tend to agree with them, but, fortunately, something can still be said:

1. at the implementation level;
2. and/or when $\mathbf{W}_i$ have special structure.

In this work we will discuss the two topics above and their usefulness in fuzzy system identification and on specific classes of LP problems tackled with IPMs.

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Approaching Lexicographic Mixed-Integer Linear Programming Problems Using Grossone Methodology

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Keywords. Multi-Objective Optimization; Lexicographic Optimization; Mixed Integer Linear Programming; Numerical Infinitesimals.

In a previous work (see [1]) the authors have shown how to solve a Lexicographic Multi-Objective Linear Programming (LMOLP) problem using the grossone-based methodology described in [2]. We have named such an algorithm GrossSimplex, since it was based on the well-known simplex algorithm.

The aim of this work is to provide an algorithm able to solve the same problem, when some or all the decision variables are constrained to be integer. We have called this problem LMILP (Lexicographic Mixed Integer Linear Programming).

This new problem is solved by introducing the GrossBB algorithm, which is the generalization of the Branch and Bound (BB) algorithm able to deal with lower-bound and upper-bound estimates which involve infinite and infinitesimal numbers (i.e., grossone-based numbers). After providing the theoretical conditions for its correctness, we show hot it can be coupled with the GrossSimplex solver described in [1], to solve the original LMILP problem. To test the correctness of the proposed algorithm we introduce a series of LMILP benchmarks having a known solution. We demostrate the ability of the GrossBB combined with the GrossSimplex to solve the proposed LMILP test problems.

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Objective and Violation Upper Bounds on a DIRECT-filter Method for Global Optimization

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Keywords. Global Optimization; DIRECT; Filter Method.

This paper addresses the problem of solving a constrained global optimization problem using a modification of the DIRECT method [3] that incorporates the filter methodology [2] to simultaneously minimize the objective function and the constraint violation. Using the filter methodology, in the "Selection" step of the herein proposed DIRECT-filter algorithm, the indices of center points of the hyperrectangles are divided into four sets and consequently separately handled. One includes the non-dominated hyperrectangles that lie in a "feasible-band" region with a sufficiently small constraint violation value, as well as the "feasible" hyperrectangle with the smallest objective function value. The other includes the dominated hyperrectangles with center points inside the "feasible-band" region appended with the remaining "feasible" hyperrectangles. The indices of "infeasible" hyperrectangles are integrated into two separate sets, one contains the non-dominated center points and the other the dominated ones.

Moreover, the new algorithm also imposes upper bounds on the objective function and constraint violation, in some of the mentioned sets of indices (not all), aiming to discard some hyperrectangles from the process of identifying the potentially optimal ones. A heuristic that avoids the exploration of the hyperrectangles that have been mostly divided is also implemented. Numerical experiments are carried out to test the effectiveness of the heuristic and the imposed upper bounds, and to compare with other available methods [1].

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The approximate synthesis of optimal control for heterogeneous discrete systems with intermediate criteria

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Keywords. heterogeneous discrete system; intermediate criteria; approximate synthesis; optimal control.

We consider one of the classes of hybrid systems: heterogeneous discrete systems (HDSs) [1]. The mathematical model of an HDS is a two-level model, where the lower level represents descriptions of homogeneous discrete processes at separate stages and the upper level (discrete) connects these descriptions into a single process and controls the functioning of the entire system to ensure a minimum of functionality. In addition, each homogeneous subsystem has its own goal.

A method of the approximate synthesis of optimal control is constructed on the basis of Krotov-type sufficient optimality conditions obtained for such a model in two forms [2, 3]. Each iteration of the method includes the solution of the vector-matrix HDS Riccati type for the first and second derivatives of the Krotov functions of both levels. The increments of the controls of both levels linearly depend on the increments of the states, which makes it possible to obtain a solution in the form of an approximate linear synthesis of optimal control.

A theorem on the convergence of the method with respect to a function is proved and an illustrative example is given.

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Modelling climate changes with stationary models: is it possible or is it a paradox?

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Keywords. Rainfall processes; Climate changes; Stationary models.

Climate is changing; many analyses of time series converge in this sentence, but this does not imply that the past is no more representative of the future, and then that "stationarity is dead". In fact, "stationarity" and "change" are not mutually exclusive. As examples: 1) according to Newton's first law, without an external force, the position of a body in motion changes in time but the velocity is unchanged; 2) according to Newton's second law, a constant force implies a constant acceleration and a changing velocity. Consequently, "non-stationarity" is not a synonymous with change; change is a general notion applicable everywhere, including to the real (material) world, while stationarity and non-stationarity only regard the adopted models. Thus, stationary models can be also adopted for environmental changes. With this aim, in this work authors show some numerical experiments concerning rainfall processes. In details, a Neymann Scott Rectangular Pulse model (NRSP, which is one of the most used for generating continuous rainfall time series) with some changing temporal scenarios for its parameters is adopted, and the derived Block Maxima time series are investigated for several temporal resolutions (sub-hourly and hourly scales). The goal is to analyze if there are some particular scales in which some sets of the assumed temporal changes in parameters could be "hidden" when Block Maxima time series (which are nowadays more available and longer than high-resolution continuous time series for many sites in the world) are studied, and then stationary models for Extreme Value distribution could be however adopted. The numerical experiments confirm that is obtained from analysis of Annual Maximum Rainfall (AMR) series in some parts of Italy, for which it is not essential to remove the hypothesis of stationary parameters: significant trends could not appear only from the observed Block Maxima data, as a relevant rate of outlier events also occurred in the central part of the last century.

An efficient optimal solution approach for the preference-based multicriteria shortest path problem with reference points

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Keywords. Multiple criteria analysis; Pareto-optimal paths; Reference point method.

The shortest path problem arises in several context, e.g., in transportation and telecommunication fields. New requirements in solving practical problems impose that more than one criterion should be considered. Since the objectives are in conflict, the solution is not unique, rather a set of (efficient) solutions is defined optimal. Among the efficient solutions, the decision maker chooses the most satisfactory. Generally, computing the entire set of efficient solutions is time consuming. Given an aspiration point, we consider the problem of finding an efficient solution that better satisfies the requirement of the decision maker [1]. This results in a max-min problem for which classical optimality principle for the shortest path problem is not valid. To overcome this issue, we propose an equivalent formulation dealing with the constrained shortest path (*CSP*) problem [2]. The idea is to define a set of constraints guaranteeing that the optimal solution to the problem at hand lies in the feasible region of the defined *CSP* problem. Then, we propose a labelling algorithm to search for the optimal solution to the *CSP* problem that is also the optimal for the problem at hand. The method is compared with the-state-of-the-art considering random and grid networks, under several scenarios.

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A Novel Geometric Approach to the Problem of Multidimensional Scaling

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Keywords. Multidimensional scaling; Geometric approach; Minimization.

Multidimensional scaling (MDS) is one of the most popular methods for a visual representation of multidimensional data [1], [2]. Low-dimensional visualization requires holding proximities between multidimensional points (observations) $X_i = (x_{i1}, x_{i2}, \ldots, x_{in})$, $i = 1, \ldots, m$, as much as possible. MDS requires estimating the coordinates of new points $Y_i = (y_{i1}, y_{i2}, \ldots, y_{id})$, $i = 1, \ldots, m$, in a lower-dimensional space ($d < n$) by minimizing some stress function. Proximity can be measured by the distance. Consider such stress: $E_{\text{MDS}}(Y_1, \ldots, Y_m) = \sum_{i<j}(D(X_i, X_j) - D(Y_i, Y_j))^2$, where D is the Euclidean distance between a pair of points. The stress function has many local minima often, and iterative algorithms are used for its minimization. Various attempts are made to find the global minimum of the stress function still now. Classical approaches to minimize the stress reached their limits. New viewpoint to the problem is necessary, including its formulation and ways of solving.

The proposed idea is based on a novel geometric interpretation of the stress function and MDS in general. Following this interpretation, the step size and direction forward the minimum of the stress function are found analytically for a separate point without reference to the analytical expression of the stress function, numerical evaluation of its derivatives and the linear search. It is proved theoretically that the direction coincides with the steepest descent direction, and the analytically found step size guaranties almost the optimal step in this direction. Moreover, regions for optimal starting points for local optimization may be disclosed. Various strategies of application of the discovered option to minimize the stress function are presented and examined. According to the experiments, the realizations of our approach tends to solve the global optimization problem.

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Finite-time stability for neural networks with time varying delay based on an improved reciprocally convex inequality

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Keywords. Finite-time stability; neural networks; time varying delay.

Finite-time stability for neural network with time-varying delay is considered by using improved reciprocally convex inequalities and some integral inequalities, which are employed to provide a tight upper bound on the time-derivative of some Lyapunov-Krasovskii functional. New sufficient conditions for finite-time stability are established to guarantee finite-time stability for the system are given in terms of linear matrix inequalities(LMIs). Numerical examples are given to illustrate the effectiveness of the obtained result.

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A Simulink-based Infinity Computer simulator and some applications

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Keywords. Infinity Computer; Numerical differentiation; Scientific Computing.

On a wide range of problems in different mathematical domains (such as numerical differentiation, optimization, divergent series, ordinary differential equations, fractals, and set theory), the results obtained by exploiting the *Infinity Computing* methodology have shown an higher accuracy respect to the results obtained by traditional tools used to work with mathematical objects involving infinity [1, 2]. In this context, the availability of software libraries able to work numerically with infinite and infinitesimal *Grossone*-based numbers can promote a wider adoption of the *Infinity Computing* and related benefits. Indeed, such software libraries can be integrated in popular scientific computational environments and platforms so as to allow a seamless exploitation of *Infinity Computing*-based algorithms and methods in solving a wide range of scientific and technological problems. To this aim, the paper presents the design and implementation of a software library for the Simulink platform that allows to represent *Grossone*-based numbers and use them in Simulink computational models. For a basic set of classical mathematical problems (including ordinary differential equations), the results obtained by using the library are compared with those achievable by using the standard Simulink functions showing a considerable increase in both accuracy and efficiency. Future research efforts will be geared to improve and extend the library as well as to exploit it for modeling and simulating complex engineered systems.

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Issues on Large Symmetric Indefinite Linear Systems and Grossone

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Keywords. Indefinite Linear Systems; Conjugate Gradient (CG); Grossone.

We are interested about investigating the effective and efficient solution of large indefinite linear systems, by means of iterative procedures. In particular, we focus on Krylov-subspace methods based on the generation of conjugate directions, which are quite appealing for their simplicity and versatility in optimization frameworks. Among them we also consider a possible extension of the Conjugate Gradient (CG) method [1], as was recently proposed in [2], for the solution of positive definite linear systems. We investigate to what extent pairing the numeral *grossone* (see [4]) with CG-based methods, may possibly deflate pivot breakdown of the CG in the indefinite case. In this regard, we use the results in [3] and we also focus on preconditioning issues, as well as on numerical performance. Finally, recalling that our main interest is for indefinite linear systems in optimization frameworks, we also study the impact of using grossone on the generation of negative curvature directions for the objective function. This latter subject is of great interest on large scale settings, since computing negative curvature directions without storing full matrices is a challenging issue.

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Non-Archimedean Game Theory and the Infinity Computer: a Numerical Approach

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Keywords. Game Theory; Prisoner's Dilemma; Non-Archimedean Payoffs and Probabilities; Infinity Computer; Grossone Methodology.

In this work we aim at generalizing Pure and Impure PD iterated games [1] when using finite/infinite/infinitesimal payoffs and finite/infinitesimal probabilities, i.e., dealing with non-Archimedean quantities (realm so far investigated only on the theoretical side, e.g. [2]). In our work we are able to generalize Pure and Impure iterated PD games, both from the theoretical and operational standpoints, by means of the Sergeyev's Infinity Computer and his Grossone Methodology [3]. Indeed, the theoretical novelties introduced have been also validated numerically in Matlab, by means of an Infinity Computer simulator.

Pragmatically, we have analytically proved that in Pure and Impure Iterated PD games involving non-Archimedean quantities, if the latter have different orders of infinite than the magnitude of the players average expectations per iteration can span all such orders (i.e., can be either infinite, finite or infinitesimal) depending on the adopted strategies. Moreover, exploiting the Infinity Computer simulator we have plot such expectations for both the PD scenarios, numerically validating the theoretical results. Finally, we have shown that the new graphic thus obtained is a generalization of the finite case, proving the maintaining of the requested properties of linearity, continuity and proper slope of its edges.

This new approach opens the door to a more precise modeling of non-Archimedean scenarios, as demonstrated in a previous work of the same authors [4]. Here, the existence and the relative numerical treatment of a new class of PD Tournaments (which previous approaches were not able to discover, nor to manage) has been demonstrated by means of such finer modeling paradigm.

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High-performance algorithms for large-scale multiobjective radiotherapy planning problems

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Keywords. Evolutionary Multiobjective Optimization; High-Performance Computing; Radiotherapy Planning; Sparse-matrix Computations.

Modern intensity-modulated radiotherapy (IMRT) equipment operates several radiation beams, each of them consisting of thousands of beamlets. The intensity of irradiation doses is controlled at the level of a single beamlet. Designing radiotherapy treatment plans (RTTPs) is often modeled as multiobjective optimization problems (MOPs). In clinical practice, solving such MOPs can be done by finding a fair, discrete representation of the set of Pareto optimal RTTPs, which represents non-dominated trade-offs between the radiation doses delivered to the tumor and these delivered to healthy organs.

Radiation doses in all the voxels (the 3D mesh of irradiated part of patient's body) represented by vector d, are evaluated using sparse matrix multiplication $d = Dx$, where D is the the dose-influence matrix specific to the patient, and x is the vector of beamlet intensities. All constraints and objectives of the MOP are defined over vectors d. The challenge is that the search space of vector x is very large, as it represents all possible geometric configurations of the irradiation system, and may contain tens of thousands of components. Due to that, classic optimization methods are inefficient.

In order to address this challenge and handle radiotherapy planning MOPs effectively, we combine preference-based evolutionary multiobjective optimization algorithms, large sparse matrix multiplication techniques, and parallel computing. The efficiency of the developed hybrid algorithms has been experimentally explored on modern high-performance computing platforms by solving real-life RTTP cases. Significant acceleration has been reported.

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A Spherical Separation Approach for Multiple Instance Learning

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Keywords. Multiple Instance Leariming; Spherical Separation; Classification.

Multiple Instance Learning (MIL) consists in classifying sets of points: such sets are called bags and the points inside the bags are called instances. The main characteristic of a MIL problem is that in the learning phase only the labels of the bags are known whereas the labels of the single instances inside the bags are unknown.

We consider the binary case whose objective is to discriminate between positive and negative bags, in the presence of positive and negative instances as well. In particular we assume that a bag is positive if it contains at least a positive instance and it is negative if all its instances are negative.

Starting from this assumption, we propose an instance-level algorithm based on the spherical separation of sets. Our approach consists in the alternation between the computation of the radius of the separating sphere when the center is fixed, and of the computation of the center when the radius is fixed.

Preliminary computational results are presented on some datasets drawn from the literature.

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Computing Stationary Equilibria in Multi-Leader-Follower Games

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Keywords. Multi-leader-follower game; equilibrium problem with equilibrium constraints; stationary equilibrium; penalty method.

In a multi-leader-follower game, there are several players who serve as leaders and the rest of players who serve as followers. As a bilevel game, all leaders compete with each other in a non-cooperative Nash game in the upper-level and make their decisions first by anticipating the responses of followers. The followers observe the leaders' decisions and then make their decisions in the lower-level with the strategies of leaders as exogenous parameters. A mathematical formulation to model the multi-leader-follower game is the equilibrium problem with equilibrium constraints (EPEC), which is a single-level equilibrium problem where each leader's optimization problem is a mathematical program with equilibrium problem (MPEC). Such an EPEC is still difficult to deal with, since the constraints of each leader's problem depend on the other leaders' strategies, and all leaders share decision variables of the followers. In this work, we propose an algorithm that combines the penalty approach for an MPEC with a diagonalization method that solves each leader's MPEC cyclically by fixing the other rival leaders' strategies. In the proposed method, each leader's MPEC is transformed into a differentiable optimization problem by means of a penalty technique, in such a way that the constraints of the problem do not depend on the other rival players' strategies. Hence it can be dealt with as an ordinary Nash equilibrium problem, where each player's problem is a nonconvex optimization problem. We show that a limit point of the sequence generated by the algorithm is an EPEC S-stationarity point under suitable assumptions.

[This talk is based on the joint work [1] with Atsushi Hori.]

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Enclosure of the Range of a Complex Polynomial Over a Complex Interval

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Keywords. Multivariate complex polynomial; Enclosure of the range; Bernstein polynomial.

Bounding the range of a function over a given region is an important task which is inherent in a remarkable variety of problems in mathematics and many of its applications. These include quantitative estimation of the remainder terms in numerical integration and differentiation, sensitivity analysis of systems, the certification of properties of function like monotonicity, convexity, and univalence, and branch and bound methods in global optimization, to name only a few. In this talk, we consider complex polynomials. The regions over which the range of such polynomials are sought are axis-aligned compact regions in the complex plane called complex intervals. The tool we are using is the expansion of the given polynomial into Bernstein polynomials, see, e.g., [1]. The convex hull of the coefficients of this expansion, the so-called Bernstein coefficients, provides an enclosure for the range of the given polynomial over the complex interval.

We first briefly recall the expansion of a multivariate real polynomial into Bernstein polynomials over a box and some of its fundamental properties as well as from [2, 3], a matrix method for the computation of the Bernstein coefficients. We present the Bernstein expansion for a complex polynomial which is applied for finding an upper bound for the modulus of a polynomial. It turns out that the computation of the range of a complex polynomial over a complex interval can be reduced to the calculation of the range over its boundary. We discuss some methods for the computation of the Bernstein coefficients of a complex polynomial and extend them to multivariate complex polynomials and to rational functions.

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MINLP formulations of the Feature Selection problem in SVM framework

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Keywords. SVM; Feature Selection; Sparse Optimization; DC function.

We consider a sparse optimization problem, where the two objectives of minimizing a convex, not necessarily differentiable, function $f : R^d \to R$, $d \geq 2$ and of keeping as small as possible the number of nonzero components of the optimal point are simultaneously pursued. Such problem is of interest in Feature Selection within the SVM (Support Vector Machine) binary classification. We adopt the following formulation:

$$f_0^* = \min_x f(x) + \|x\|_0, \tag{1}$$

where the symbol $\| \cdot \|_0$ indicates the ℓ_0 pseudo-norm, which counts the number of nonzero components of any vector.

A "big M" reformulation of the problem is easily obtained by introducing a set of binary variables counting the sparsity of vector x.

Our alternative approach [1] is based on using a class of polyhedral norms known as k-norm and indicated by $\| \cdot \|_{[k]}$, $k = 1, \ldots, d$. In fact $\|x\|_{[k]}$ is the sum of the k largest components (in modulus) of x. The following property holds:

$$\|x\|_\infty \leq \|x\|_{[1]} \leq \|x\|_{[2]} \leq \ldots \leq \|x\|_{[d]} = \|x\|_1$$

The approach we use [2], is based on the equivalence, valid for $1 \leq k \leq d$,

$$\|x\|_0 \leq k \quad \Leftrightarrow \quad \|x\|_1 - \|x\|_{[k]} = 0,$$

which allows us to obtain a Mixed Integer Nonlinear Programming (MINLP) formulation of problem (1). We focus on the solutions provided by the continuous relaxations of the two above mentioned formulations. In particular the proposed approach benefits from the use of DC (Difference of Convex) optimization.

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Multidimensional global search using numerical estimations of minimized function derivatives and adaptive nested optimization scheme

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Keywords. Multiextremal optimization; global search algorithms; Lipschitz condition; numerical estimations of derivative values; dimensionality reduction; numerical experiments;

This paper reviews combination of novel approaches for solving the multidimensional multiextremal problem – the adaptive method with numerical derivatives for solving one-dimensional problems and adaptive nested optimization scheme for dimensionality reduction. The considered method uses not only the minimized function values but also the values of derivatives of these functions to increase the efficiency of global optimization, while the adaptive scheme enables to develop methods of the global optimum search, which are more efficient in comparison with the ones on the base of the usually used nested optimization scheme. The descriptions of the method and its computational scheme are provided. Results of numerical experiments on the well-known classes of the test multiextremal functions confirm the developed approach is promising.

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On a Family of Fourth-order Simple-root Finders

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Keywords. fourth-order convergence; optimal order; basin of attraction.

In this paper we develop a family of two-point optimal [1] fourth-order methods that make use of one function and two derivatives for a simple-root finding problems. The proposed method is described by using the weighting functions. The convergence analysis [2] regarding proposed scheme is proved through a various numerical examples and their basin of attraction [3, 4].

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Convex Optimization for Structured Matrix Completion

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Keywords. Matrix completion, Forecasting, Big data

Matrix completion has been one of the breakthrough areas of mathematics in recent years. One can impute the missing values of a matrix with extremely high probability by solving a convex optimization problem. This is because observed data often belongs to some low dimensional subspace. Existing technology for matrix completion assumes: (i) the missing values appear randomly throughout the matrix and (ii) the non-missing values are recorded without error. It is these two assumptions which have restricted the application of matrix completion for substantive statistical problems.

This talk is motivated by the problem of forecasting. In this scenario the non-missing values are almost certainly recorded with error, and the missing values are not spread randomly throughout the matrix (but are contained in the bottom right hand corner of a structured matrix). This is known as structured matrix completion. We consider convex relaxations for the structured low-rank matrix completion problem with specific application to forecasting time series. Low rank optimization problems are known, in general, to be difficult global optimization problems, see [1] and [2] for example.

This is a fashionable approach in the statistics of big data: difficult non-convex optimization problems are 'convexified' to make them tractable. The question then is: how close is the solution of the convex optimization problem to the non-convex one (which is the one we really want to solve)? A full description of the work is available in [1]

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Adaptive Nested Multiextremal Optimization in Accessible Region with Computable Boundaries

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Keywords. Multiextremal problems; dimensionality reduction; computable boundaries.

The paper considers multidimensional optimization problems with multiextremal objective functions over search domains determined by constraints which form a special type of domain boundaries called computable ones and, in general case, are non-linear and multiextremal. The regions of this class can be complicated sufficiently including non-convex, nonsimply connected, and even disconnected domains. For solving such problems a new global optimization technique based on the adaptive nested scheme [1] developed recently for unconstrained optimization is proposed. This scheme follows the dimensionality reduction approach in the framework of which instead of solving a multidimensional problem a set of reduced univariate subproblems connected recursively is solved. The suggested optimization algorithm is a generalization of the method [2] which applied the classical nested reduction for global optimization problems over regions with computable boundaries. The advantages of the adaptive nested scheme over the classical one consist in more efficient use of new information about the solved problem obtained in the course of optimization, because for planning the search the adaptive scheme takes into account the data from all one-dimensional subproblems, whereas the classic prototype during solving a current subproblem ignores the information of the subproblems completed earlier [3].

For efficiency estimation of the proposed algorithm built on the base of adaptive nested scheme in comparison with the classical nested optimization and the penalty function method a representative numerical experiment on the test class of multidimensional multiextremal functions was carried out. The results of the experiment demonstrate the significant advantage of the adaptive scheme over its opponents.

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Fluid Flow and Meniscus Behavior during Horizontal Single Belt Casting (HSBC) of Aluminum Strips

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Keywords. Computational Fluid Dynamic; Strip Casting; Aluminum.

Horizontal Single Belt Casting (HSBC) is a green process, potentially capable of replacing the current, conventional, Direct Chill (DC) casting for aluminum alloys, as well as Thin Slab Casting (TSC) for steel. HSBC is a novel, friction-free, near-net-shape continuous casting process, with significant high cooling capability. Because of high cooling rates, the HSBC strips have reduce structural anisotropy, and reduce micro-and macro-segregation of elements within the strip product. The HSBC involves direct contact of liquid metals with cooling substrate. The quality of strips produced via the HSBC process are directly dependent on: fluid flow behavior within the delivery system, the shape of the metal delivery system, the texture of the cooling substrate, the meniscus behavior at the quadruple point of contact between melt/cooling substrate/air/refractory-containing-material, and most importantly, the interfacial heat transfer between the melt and cooling substrate. As such, High Performance Computational Fluid Dynamic modelling is the most suitable way to investigate the effect of these various conditions on the strips product quality.

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Novel criteria for finite-time stability, dissipativity, and passivity analysis of discrete-time neural networks with time-varying delays

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Keywords. Finite-time Stability, dissipativity and passivity analysis, Lyapunov-Krasovskii functional.

This paper is improved finite-time stability, dissipativity, and passivity condition of discrete-time neural networks with time-varying delays. The neural network time-varying delay is obtained. A delay-dependent condition is provided to ensure the considered discrete-time neural networks with time-varying delays to be finite-time stability, dissipativity, and passivity. An effective of LMI approach is proposed to derive the finite-time stability, dissipativity, and passivity criterion. The new Lyapunov-Krasovskii functional constructing to a novel sufficient criterion on finite-time stability, dissipativity, and passivity of the discrete-time neural networks with time-varying delays.

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A dynamic precision floating-point arithmetic based on the Infinity Computer framework

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Keywords. Infinity Computer; floating-point arithmetic; conditioning.

The Infinity Computer paradigm is based on a positional numeral system with the infinite radix ① (called grossone) representing, by definition, the number of elements of the set of natural numbers $\mathbb{N}$ [1,2]. A number in this system is a linear combination of powers of ① (grosspowers) with coefficients in the standard numeral system. Of particular interest in our study are grossnumbers consisting of a finite expansion of integer grosspowers such as, for example,

$X = ①^P \sum_{j=0}^{T} x_j ①^{-j}$, with grossdigits $x_j = \pm\beta^p \sum_{i=0}^{t} d_{ij}\beta^{-i}$, where $P, p \in \mathbb{Z}$ and T, t are given positive integers, while β stands for the base of the traditional floating-point arithmetic system (usually $\beta = 2$).

This representation suggests interesting applications of the Infinity Computer if now ① is allowed to assume a suitable prescribed finite value. The idea is to exploit the grossdigits x_i in order to store a large number of significant digits in a dynamic manner during the execution of an algorithm. This means that the accuracy may be increased/decreased on demand during the flow of computations by automatically activating/deactivating a number of negative grosspowers. Our study explores this path of investigation and is addressed to the accurate solution of ill-conditioned/unstable problems [3, 4]. It should be noticed that, in principle, neither the user nor the programmer needs to know what the value of ① actually is. This assumption should be instead understood as an inherent feature of the machine architecture which, consistently with the Infinity Arithmetic methodology, will perceive the negative powers of ① as infinitesimal-like quantities if related to the classical floating-point system.

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Ensemble Modeling for Minimization of Noisy Expensive Functions

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Keywords. Self Organizing Map; Ensemble Modeling; Stochastic Optimization, Noisy Function.

In nonlinear regression, avoiding over- and underfitting is always an issue, particularly when the sample size is small. Furthermore, estimating a minimum of the underlying function is affected by the regression (surrogate) model. This paper shows first results of fitting multiple surrogates to a noisy function using Self-Organizing Map Based Adaptive Sampling (SOMBAS) [1] and sampling new points based on the values returned by these surrogates using Differential Evolution [2, pp. 38,39]. The proposed approach does not require the selection of suitable model complexity (e.g. polynomial order). Furthermore, it does not require matrix (pseudo) inverses to fit the surrogate models nor to find its minimum (on average) points. Our initial results show that the new method effectively avoids over- and underfitting, and can estimate the minimum of an underlying function. We assume that we know the responses are noisy (e.g. expected measurement error) but we do not know the underlying function. The novelty here is that we do not aim at the least-square error but allow a threshold error tolerance below which a surrogate is supposed to achieve. The diversity of surrogates is expected to automatically cancel out the variance component to avoid over-fitting, even though we do not know the complexity (e.g. polynomial order) of the underlying function. We use statistical information of responses to adaptively sample new points for the purpose of narrowing down parameter estimate uncertainties or inferring an optimal point (an input that generates the minimum average of responses). This work was part of the Ph.D. thesis [3], but has not been published in journals nor in conference proceedings.

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Noise-induced kinetic transition in two-component environment

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Keywords. Grossone; noise-induced nonequilibrium phase transitions; percolation theory.

Over the past 30 years, noise-induced nonequilibrium phase transitions have occupied a special place in nonlinear dynamics and statistical physics. The presence of noise can not only reduce, but, on the contrary, significantly increase the sensitivity of systems to weak external influences and lead to the appearance of dynamic modes, the realization of which in the absence of noise is impossible. In systems where the interacting components have contrasting properties (significantly different mobilities, diffusion coefficients, lifetimes), the addition of noise leads to the effect of subthreshold reproduction with the redistribution of the "resource" components (deposition) and is accompanied by a significant decrease in the generation threshold of complex (most often fractal) dissipative structures compared to systems without noise [1]. Recently [2] a number of traditional models related to the percolation theory have been considered by means of a new computational methodology [3] that does not use Cantor's ideas and describes infinite and infinitesimal numbers in accordance with the principle "The whole is greater than the part" (Euclid's Common Notion 5). Here we apply this methodology to the noise-induced kinetic transitions in multicomponent distributed systems.

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Effect of Education Campaign on Mathematical Model SEIR for Controlling the Spread of Chickenpox

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Keywords. Mathematical model; Chickenpox; Control the spread; Education Campaign.

The objective of this research is to develop and evaluate stability of mathematical modelling for controlling the spread of Chickenpox on Education Campaign. The model is analysed using standard methods, the equilibrium point, stability of the equilibrium points and analytic solutions. The effectiveness of Education Campaign (ω) in mathematical modelling and numerical solutions of basic reproductive number (R_0) is studied.

The analysis model found that the stability of equilibrium points when the effectiveness of Education Campaign $\omega = 0.5$, have basic reproductive number $R_0 = 0.914$, and the effectiveness of Education Campaign $\omega = 0$, then the basic reproductive number $R_0 = 1.827$. The effectiveness of Education Campaign is the factor affecting to the mathematical modelling. If the risk of infection's population has Education Campaign and follow hypothesis increase then the spread of Chickenpox decreased until no epidemic.

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Constant-factor approximations for generalizations of the asymmetric Vehicle Routing and Traveling Salesman Problems

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Keywords. Asymmetric TSP; the triangle inequality; constant-factor polynomial time approximation.

The Traveling Salesman Problem (TSP) and Vehicle Routing Problem (VRP) are well-known combinatorial optimization problems having numerous valuable practical applications in operations research. Both problems along with their various modifications and generalizations are strongly NP-hard and remain intractable even in the Euclidean plane.

Although, all these problems are inapproximable as well in the general case, their metric settings defined by edge-weighted (indirected) graphs, whose weights satisfy the triangle inequality, can be approximated efficiently within constant factors, whilst their Euclidean settings admit Polynomial Time Approximation Schemes (PTAS) for any fixed dimension of the underlying space. As a rule, approximation algorithms developed for all these problems are based on the celebrated Christofides-Serdyukov 3/2-approximation algorithm for the metric TSP.

Meanwhile, for the Asymmetric Traveling Salesman Problem (ATSP), the question on polynomial time approximability within a constant ratio remained open for decades.

In this paper, relying on the long-awaited approximation result presented in [1] for the ATSP, we propose novel constant-factor approximation algorithms for several relevant generalizations of the ATSP and Asymmetric VRP.

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Exact Parameterized Linear-Time Algorithm for K-Means Problem with Optimized Number of Clusters for the 1D Case

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Keywords. Partition, set, one dimensional case, parameterized, optimized number of clusters, exact algorithm, linear-time.

In the well-known [1] clustering *K-Means* problem, an N-element set $\mathcal{Y}$ of points in d-dimension Euclidean space and a positive integer K are given. It is required to find a partition of the input set $\mathcal{Y}$ into K non-empty clusters minimizing the sum over all clusters of the intracluster sums of squared distances between the elements of each cluster and its centroid (geometrical center). *K-Means* problem is relevant, for example, to statistics, computational geometry, data mining, and data analysis.

It is known that this problem is strongly NP-hard in the general case [2] when the space dimension is a part of the input. But in the one-dimensional case, this problem is polynomially solvable [1]. The running time of the algorithm presented in [1] is linear on K and quadratic on N.

In [3], it was shown that if the input points are ordered, then the problem is solvable in a time that is linear both on K and N. Note that one can obtain the same running time using the approach presented earlier in [4].

Unfortunately, in the case when the number of clusters is optimized, the solution of *K-Means* problem is trivial, i.e., the number of clusters is equal to the number of points. In this paper, we present a new approach to this case. Namely, we consider some parameterized modification of *K-Means* problem and propose an algorithm that allows one to find an optimal partition as well as an optimal number of clusters in linear time.

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Polynomial-Time Approximation Scheme for a Problem of Searching for the Largest Subset

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Keywords. Euclidean space; largest subset; quadratic variation; NP-hard problem; polynomial-time approximation scheme.

In the paper, we consider a problem of searching for the largest subset in a given finite set of points in Euclidean space. The sum of squared distances between the elements of this subset and its unknown centroid (geometrical center) must not exceed a given value, which is defined as percentage of the sum of squared distances between the elements of the input set and its centroid. The problem is relevant, in particular, in Data mining, Data cleaning, Data reduction, statistics. The essence of the problem considered is searching for the largest well-concentrated subset of points.

In [1], it was shown that this problem is strongly NP-hard. In the same paper, a polynomial-time 1/2-approximation algorithm was presented for the problem.

An exact algorithm for the case of integer-valued input points was proposed in [2]. If the space dimension is bounded by some constant, the algorithm runs in a pseudopolynomial time.

In this paper, we improve the result of [1] and propose a polynomial-time algorithm for the problem with relative performance guarantee greater than 1/2. We prove that our algorithm implements a polynomial-time approximation scheme.

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On a comparison of several numerical integration methods for ordinary systems of differential equations

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Keywords. finite difference formulas, integration strategies, optimal strategy

The paper considers the numerical integration methods for ordinary systems of differential equations that have the end of the integration interval undefined a priori but defined during the integration process instead. Moreover, the calculation of right parts of such systems is expensive procedure.

The paper describes a new integration strategy based on implicit fourth order method [1]. The proposed strategy uses the behavior of obtaining solution to control the integration process. Let us remark that at every fixed interval the number of integration nodes selected by the mentioned method is minimal under the limitations defined by the local error occurring as a result of approximation of system derivatives [1]. Denote by α_1 the developed strategy.

In order to evaluate the effectiveness of the proposed strategy α_1 it was compared with `ode45` and `ode15s` methods provided in MATLAB. Below these methods will be called α_2 and α_3 respectively. The compared methods were evaluated using the following criteria. The first criterion is the number N of integration nodes, the second criterion is the number N_1 of right part calculations of the system at the integration interval and the third criterion is the maximum of difference δ of exact solution and approximate solution of test (model) problems for each solution component at every integration node. A variety of experiments was carried out on a range of model problems. It was identified that α_1 strategy shows better results (according to criteria mentioned above) on low tolerance. One of model problems used in experiments is a third-order linear system [2]. Results of α_1 were $N = 19$, $\delta = 0.02$, $N_1 = 39$, results of α_2 – $N = 20$, $\delta = 0.05$, $N_1 = 51$, results of α_3 – $N = 57$, $\delta = 0.09$, $N_1 = 81$.

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On Polyhedral Estimates of Reachable Sets of Discrete-Time Systems with Uncertain Matrices and Integral Bounds on Additive Terms

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Keywords. Discrete-time systems; reachable sets; uncertain matrix; integral constraints; polyhedral estimates.

The reachability problem is one of the fundamental problems of the control theory [1]. Since exact construction of reachable sets is usually a very complicated problem, different numerical methods are developed, in particular, methods based on estimating sets by domains of simple shape such as ellipsoids [1, 2], parallelepipeds [3, 4], which are not too computationally demanding.

The research is devoted to estimating reachable sets of bilinear discrete-time (difference) systems with integral non-quadratic constraints on additive terms, where the bilinearity is caused by uncertainty in coefficients of the system under interval constraints. We present techniques for constructing external and internal polyhedral estimates in the form of parallelepipeds, parallelotopes and special polytopes. The main attention is paid to internal estimates. The approach described in [3] for linear time dependent systems is expanded to the more complicated case of bilinear systems, which have properties of nonlinear ones (in particular, reachable sets can be non-convex). Also we present novel (in comparison with [4]) primary internal estimates for the result of multiplying an interval matrix on a parallelotope. The constructed estimates can be used for obtaining estimates of reachable sets for impulsive differential systems [2].

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Numerical Investigation Of Natural Rough-Bed Flow

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Keywords. Gravel bed flow; Large Eddy Simulation; Volume of Fluid.

The turbulent flow in natural rough-bed watercourses is a rather complex phenomenon, still poorely investigated. The majority of the existing works on this subject are of experimental nature, while the numerical ones are mostly related to artificially and regularly roughened beds. In the present work a nu- merical investigation is carried out, in which the fully turbulent flow in an open channel is simulated, where the channel bottom is constituted by natural-pebble layers. In the numerical simulations, the LES approach is used (Large Eddy Sim- ulation), in conjunction with the WALE (Wall-Adapting Local Eddy viscosity [1]) SGS closure model (Sub-Grid Scale) at Reynolds number 46500 and Froude number 0.186. For the simulations, the pebble-bed surface has been captured from the bottom of a laboratory flume with a high-resolution 3D laser scanner, and used to morphologically characterize the bottom of the numerical channel. The Finite-Volume discretized governing equations are solved numerically by means of the InterFOAM solver, embedded in the OpenFOAM C++ libraries. In order to take into account the free-surface dynamics, the VoF (Volume of Fluid) method is used. A CPU-based computational system has been used for the computations. The system included one worker node equipped with two 8- core Intel E5-2640 CPUs (a total of 16 cores/16 threads at 2.0 GHz), 128 GB RAM at 1899 MHz, and 4 TB disk space. The code has been parallelized through the public domain OpemMPI implementation of the standard Message Passing Interface (MPI). The results of the simulations are compared with those ob- tained in a companion experiment [2] mainly in terms of turbulence statistics of different orders, obtaining a rather good agreement. Moreover, the vorticity field has been visualized using the relation between vorticity and Turbulent Kinetic Energy (TKE) dissipation [3].

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Numerical Simulation Of Ski-Jump Hydraulic Behavior

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Keywords. Ski jump, RANS modeling, OpenFOAM toolkit.

The hydraulics of ski jumps is an issue of great importance in dam construction, the former being in practice the only existing solution as related to the dissipation of energy from high-speed spillway flows from large dams. Inspite of the fact that thousands of dams have been built all over the world in the years, and besides the reporting of specific case studies, the general hydraulic behavior of the ski jumps has been scarcely investigated. In the present work, the hydraulic behavior of ski jumps is investigated numerically using the OpenFOAM digital library [1]. A number of ski-jump cases has been simulated numerically following the RANS (Reynolds Averaged Navier-Stokes equations) approach, using the kappa-omega SST closure model [2] and ther VoF technique (Volume of Fluid) for the tracking of the flow free surface [3]. The numerical procedure appears to be a rather favourable option to overcome the complexities always associated to experimental measurements. Particular attention is given to the forces, to the pressure distribution in the zone of impact of the falling jet, and to the length of the jet itself. The issue of the length of the falling jet is particularly considered, as defined as the distance along the x- direction between the point of maximum dynamic pressure head in the zone of impact of the jet along the centerline of the tailwater channel, and the origin of the reference system. A chart is proposed, reporting the correlation lines (and correspondent formal expressions) between the approach Froude numbers and the lengths of the jets, in the limit of the range of other parameters tested. The chart may serve as a useful tool to determine the length of the jet taking off from the bucket, starting from the value of the approach Froude number.

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Approximating the solution set of nonlinear inequalities by using Peano space-filling curves

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Keywords. Nonlinear inequalities; space-filling curves approximations; Lipschitz constant.

In this paper we study an algorithm for solving systems of nonlinear inequalities coming from practical applications (see [1, 2]) that uses a non-uniform covering approach of the domain, that generates inner and outer approximations of the solution set. In particular, we propose a method that uses one of the mostly abstract mathematical objects, the space-filling curves introduced by Peano in 1890 and independently by Hilbert in 1891 (see [3,4]). The main idea consists of the reduction of the dimension of the initial problem in order to pass from a multivariate problem to a univariate one in which we use the Peano curves to pass from a domain in N dimension to a one-dimensional interval. That is, the proposed method builds a coverage of the domain in N dimensions going to work in the interval $[0,1] \subset \mathbf{R}$. Finally, we apply the methods to find the working area of some parallel robots.

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Numerical simulation of Hyperbolic conservation laws using high Resolution schemes with the indulgence of Fuzzy logic

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Keywords. Conservation laws; fuzzy logic; limiters.

In this paper we apply some fuzzy operators to reconstruct several higher order numerical methods to solve problems in Hyperbolic Conservation laws including the high resolution total variation diminishing (HR-TVD)methods and some very high order finite volume methods for scalar conservation laws . High resolution methods are significant for hyperbolic conservation laws because of better results as compared to the first generation methods which are in general, least concerned with the initial solution. So, in order to avoid this drawback various strategies have already been given by many researchers like Van Leer, Sweby, Roe etc. In this paper we introduce these high resolution methods using a different approach based upon the optimization of existing high resolution methods using fuzzy logic. Mainly, in our work, we target a few applications using some fuzzy logic features in order to enhance the quality of existing numerical solutions via some standard test problems. Further, we discuss the application of our work by demonstrating the performance of these optimized schemes as compared to the popular numerical schemes in existing literature.

Acknowledgements.

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General framework for binary nonlinear classification on top samples

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Keywords. Binary classification; duality; kernels; accuracy at the top; ranking; hypothesis testing.

In our previous work [1], we have proposed a general framework to handle binary linear classification for top samples. Our framework includes ranking problems, accuracy at the top or hypothesis testing. We have summarized known methods, such as [2–4], belonging to this framework and proposed new ones. Note that these methods were either derived in their primal form, or they did not use kernels. This forced a restriction on only linear classifiers.

In this work, we employ the convexity results derived in [1]. For all methods from our framework, we derive their equivalent dual formulation. We utilize their SVM-like structure and incorporate kernels into the dual formulation. This allows us to pass from linear to nonlinear classifiers. We show how to recover the primal solution and classification value for new samples. We propose an effective computation method and perform a numerical analysis showing the efficiency of our framework.

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On Faber's type decomposition for minimal spline spaces

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Keywords. Splines; wavelets; nonuniform knots; multiresolution analysis.

Splines and wavelets are widely used in information theory. Wavelet decompositions are connected with developing efficient algorithms for processing (e. g. compressing) huge digital data flows. One of the simplest and the most common processing schemes for such arrays is piecewise linear interpolation on uniform grids. It is well known if this scheme is used as a basis for multiresolution analysis, then it is often referred to as Faber decomposition. Faber decomposition has many attractive features from a computational perspective. It leads to decent compression, it is fast and simple in implementation.

We construct new types of Faber decomposition for spaces of minimal splines constructed on nonuniform grids on segment. The approach is based on development of algorithms of spline wavelet decomposition [1] uses approximation relations as an initial structure for constructing the spaces of minimal splines. These splines [2] as a special case include well known polynomial B-splines and share most properties of B-splines (linear independency, smoothness, nonnegativity, etc.). In the particular case of B-splines this approach (providing a lifting scheme in the general case) leads to constructing either lazy wavelets or wavelets with mixed supports [3]. The advantages of this approach are the possibilities of using nonuniform grids on segment and sufficiently arbitrary nonpolynomial spline wavelets.

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Methodology for interval-valued matrix games with 2-tuple fuzzy linguistic information

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Keywords. 2-tuple fuzzy linguistic model; Interval-valued 2-tuple fuzzy linguistic model; Interval-valued linguistic linear programming method.

The 2-tuple fuzzy linguistic model formalized by Herrera and Martinez [1] represents linguistic information via 2-tuple i.e. (ℓ_i, α_i) where ℓ_i belongs to a linguistic term set and $\alpha_i \in [-0.5, 0.5)$. Zhang [2] further extended this model to propose interval-valued 2-tuple fuzzy linguistic (IVTFL) model. There is wide and extensive existing literature based on IVTFL approach and its application in problems of decision-making and other distinct fields. Game theory is one such application area where the fuzzy framework has shown progress and fuzzy linguistic game theory is pristine to deal with uncertainty. In this paper, we consider a non-cooperative 2-player constant sum IVTFL matrix game and develop a method to solve such class of IVTFL matrix game. For this, we have constructed an interval-valued linguistic linear programming (IVLLP) problem which is then transformed into interval linear programming (ILP) problem. Our objective is to obtain a strategy set of IVTFL game problem as the region which is not only completely feasible, but also totally optimal. The hypothetical example further implements the methodology to illustrate the expertise of the proposed method in the real world. Finally, the results are compared with the Best-Worst Case (BWC) method [3], Enhanced-Interval linear programming (EILP) method [3] and interval-valued linguistic linear programming (IVLLP) method [4].

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Molecular Dynamics Performance Evaluation With Modern Computer Architecture

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Keywords. Gromacs; High Performance Computing; Molecular Dynamics.

Ligand-based control of protein functional motions can provide fresh opportunities in the study of fundamental biological mechanisms and in the development of novel therapeutics. A prototypical example is represented by integrin avb6, a transmembrane protein with promising anticancer properties. Despite the simplicity of the ligand-based model, fundamental mechanisms that regulate these interactions are poorly understood.

An adequate equipment is mandatory to unravel this scientific challenge, not only through cost savings but also with high-quality results. With this in mind, we performed Molecular Dynamics simulations using the Gromacs package (version 2018.3) on two promising platforms: Cavium ThunderX2 ARM based servers[1] and Shared-memory Intel based single-node machines[2].

The performance test consisted in a solvated integrin avb6 complex with TGF-β peptide using the X-Ray crystal structure [1] for the system preparation. Aforementioned tests were also performed on common Intel based servers[3] as a reference.

Acquired results shown that shared-memory machine is the fastest in our pool, mainly due to the higher clock frequency of its CPU. This being said, performance differences are significantly reduced with the increment of employed resources (i.e. number of sockets). As a matter of fact, ARM and Intel servers turned out to be as fast as Shared-memory machine when more than four sockets are adopted. This can be explained by the fact that Gromacs code does not take full advantage of the absence of network interfaces in the single-node setup.

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[2] One server equipped with eight Intel Xeon® Platinum 8168 and 1.5 TB of memory at 2666 MHz
[3] Four servers equipped with two Intel Xeon® Gold 6130, 96 GB of memory at 2400 MHz and Mellanox ConnectX5 EDR interface.

Existence and uniqueness of time-fractional diffusion equation on a star graph

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Keywords. Time-fractional diffusion equation; Caputo fractional derivative; Weak solution.

Mathematical modelling in different fields of science and engineering such as processes on the nets of gas pipeline [2], controlled vibrations of networks of strings [1], water wave propagation in open channel networks [4] naturally lead to partial differential equation on graphs. In this paper, we consider a time-fractional diffusion equation on a star graph. We investigated the existence and uniqueness of the weak solution based on eigenfunction expansions [3]. Some priori estimates and regularity results of solution are also proved.

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Handling Ill-Conditioning in Some Optimization Problems via Infinity Computing

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Keywords. Lipschitz Global optimization; univariate problems; Infinity Computing

This contribution is dedicated to several issues of ill-conditioning in optimization and its handling by using numerical infinities and infinitesimals. First, scaled univariate Lipschitz global optimization problems are considered (see, e.g., [4]). In this case, numerical solution to the scaled problems can lead to incorrect results due to underflows and overflows if the traditional computational architectures are used (see, e.g., [3, 3]). Second, ill-conditioning in multidimensional variable metric methods produced by discontinuity in the derivatives is also studied (see, e.g., [4]). It is shown that both the instances of ill-conditioning can be successfully resolved by using the Infinity Computing framework. Experimental results on several classes of test problems taken from the literature using a software simulator of the Infinity Computer confirm that the proposed techniques can be successfully used in practice.

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On the Exact Higher Order Differentiation Techniques on the Infinity Computer

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Keywords. Numerical differentiation; High-Precision Computing; Infinity Computing

In this contribution, several techniques of the exact higher order numerical differentiation are presented for the Infinity Computer – a new type of a supercomputer that is able to work *numerically* with finite, infinite and infinitesimal numbers in a unique framework (see the patents [3] and the detailed description of the methodology in [4]). The objective function is considered to be given as a computational procedure unknown to the user, i.e., given as a "black-box" (see, e.g., [3]). Then, techniques for the exact differentiation of the function of interest given implicitly as a solution to an ordinary differential equation are also presented (see, e.g., [4]). It should be noted that the presented techniques are *numerical* and not *symbolic* giving so the possibility to calculate exactly the higher order derivatives using floating-point numbers. Moreover, it is shown that the presented techniques are efficient and much simpler and faster than symbolic ones.

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Set-membership computation of integrals with uncertain endpoints

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Keywords. Integral; Set-membership Computation; Interval Methods.

Numerical integration is one of the fundamental tool of scientific computation. Providing a reliable result to such problem is important for validated simulation [1] or for global optimization with continuous objective function [2]. An important work on inclusion methods for integral equations can be found in [3]. We propose an efficient **guaranteed** method for the computation of the **integral** of a nonlinear continuous function f between two **interval endpoints** $[x_1]$ and $[x_2]$, define by:

$$\int_{[x_1]}^{[x_2]} f(x)dx = \left\{ \int_{x_1}^{x_2} f(x)dx \, : x_1 \in [x_1]\,, x_2 \in [x_2] \right\} \tag{1}$$

Two cases can occur whether the intervals $[x_1]$ and $[x_2]$ intersect or not. If the two intervals do not intersect, we produce an outer approximation of the set of possible values for the integral proving the following proposed theorem:

Theorem 1. *Let $f : \mathbb{R} \to \mathbb{R}$ be a differentiable function. For $[x_1] = \left[\underline{x_1}, \overline{x_1}\right]$ and $[x_2] = \left[\underline{x_2}, \overline{x_2}\right]$ two intervals in $\mathbb{IR}$. Then the minimum and the maximum of set* (1) *can be defined by*

$$\int_{[x_1]}^{[x_2]} f(x)dx = \left[\min \int_{\mathcal{X}^*_{1-} \cup \{\overline{x_1}\}}^{\mathcal{X}^*_{2+} \cup \{\underline{x_2}\}} f(x)dx, \max \int_{\mathcal{X}^*_{1+} \cup \{\overline{x_1}\}}^{\mathcal{X}^*_{2-} \cup \{\underline{x_2}\}} f(x)dx \right] \tag{2}$$

using
$\mathcal{X}^*_{i-} = \{x \in [x_i] : f(x) = 0, f'(x) < 0\}$, $\mathcal{X}^*_{i+} = \{x \in [x_i] : f(x) = 0, f'(x) > 0\}$.

When the two intervals intersect, Second Fundamental Theorem of Calculus is applied. An implementation of the computation of the bounds (2) is introduced using interval analysis [4] and tested on several examples.

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On Acceleration of Derivative-Free Univariate Lipschitz Global Optimization Methods

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Keywords. Lipschitz Global optimization; univariate problems; derivative-free optimization

In this contribution, univariate box-constrained global optimization problems, where the objective function is supposed to be Lipschitz continuous and multiextremal on the search interval are considered (see, e.g., [1]). It is supposed also that the analytical representation of the objective function is unknown, i.e., it is given as a "black-box", and even one its evaluation is a computationally expensive procedure (see, e.g., [2]). Geometric and information statistical frameworks for construction of global optimization algorithms are discussed (see, e.g., [3,4]). Several powerful acceleration techniques are briefly described. Numerical experiments on broad classes of test problems taken from the literature show advantages of the presented techniques with respect to its direct competitors.

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On simplicial distances with a view to applications in statistics

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Keywords. Cluster analysis, Mahalanobis distance, Large dimension

The authors of [1] have introduced the following family of the so-called 'simplicial outlyingness functions' computed for a sample X_N of d-dimensional data:

$$O_k(x) = \frac{1}{k}\left\{e_k\left[\Lambda\left(\Sigma_N + (x-a)(x-a)^T\right)\right] - e_k\left[\Lambda\left(\Sigma_N\right)\right]\right\}$$

where $x \in R^d$, $k = 1, 2, \ldots, d$, Σ_N is an empirical covariance matrix constructed from the sample X_N, $\Lambda(A)$ is a set of eigenvalues of a symmetric matrix A, a is the sample mean (which can be assumed to be zero) and e_k $(k = 1, 2, \ldots, d)$ is a symmetric functions of order k. The k-th order simplicial Mahalanobis distance between $z_1, z_2 \in R^d$ relative to the given sample is then $O_k(z_1 - z_2)$.

As shown in [1], the simplicial Mahalanobis distance is proportional to the sum of squared volumes of all simplices formed by vector x and all k-tuples of the sample X_N. If $k = 1$ then $O_k(z_1 - z_2)$ is the standard Euclidean distance but $O_d(z_1 - z_2)$ turns into the Mahalanobis distance between z_1 and z_2.

As is well-known, the Mahalanobis distance is one of the key tools in applied statistics. However, it cannot be used when the data is degenerate; that is, lies very close to a lower-dimensional subspace of R^d. We will demonstrate that in such situations the simplicial distance with an appropriate choice of k would be a very good substitute for the Mahalanobis distance.

Applications in classification and cluster-analysis problems are given.

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Parallel Algorithms for Convex Mixed-Integer Nonlinear Optimization

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Keywords. shared-memory parallel; branch-and-cut; convex MINLP

Exact algorithms for solving convex mixed-integer nonlinear programs (MINLPs) [1] are based on branch-and-bound. We implement parallel extensions of two such algorithms in a multi-threaded shared-memory architecture. First is the nonlinear programming (NLP) based branch-and-bound. Here, multiple threads of our process solve different NLP subproblems of the tree in parallel. We also develop a parallel extension of the LP/NLP based branch-and-bound [1]. This algorithm creates a mixed-integer linear programming (MILP) relaxation of the original MINLP using linear outer approximation of the nonlinear constraints and objective function. Multiple threads in our implementation solve different LP subproblems of the tree in parallel. Both these algorithms are available in the open-source MINLP toolkit, MINOTAUR [2].

We briefly describe subroutines critical for parallel versions of these algorithms: branching, node-selection, cut generation, warm-starting and heuristics. Since these techniques rely on information collected at various stages of the algorithm, we need to effectively share the updated information across all threads. While some information like globally-valid cuts, pseudo-cost scores for branching and the incumbent solution are useful globally, other information like updated bounds, presolve information etc. are only locally useful. A parallel version of reliability brancher is presented. Effective tree search strategies and heuristics that run in parallel are tested under various settings on the MINLP Library. MILP solvers that exploit parallelism can be used in a third algorithm called outer-approximation (OA). We compare the empirical performance of OA using a multi-threaded MILP solver as a black-box to the LP/NLP algorithm using multithreaded single tree search.

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An Approximation Polynomial-Time Algorithm for One Hard-to-Solve Weighted 2-Partitioning Problem of a Sequence

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Keywords. Euclidean space; sequence of points; weighted 2-partition; quadratic variation; NP-hard problem; approximation algorithm; polynomial time.

We consider a problem of 2-partitioning a finite sequence of points in Euclidean space into clusters of the given sizes with some constraints. The solution criterion is the minimum of the sum of weighted intracluster sums of squared distances between the elements of each cluster and its center. The weight of the intracluster sum is equal to the cluster size. The center of one cluster is given as input (is the origin without loss of generality), while the center of the other one is unknown and is determined as a geometric center. The following constraints hold: the difference between the indices of two subsequent points included in the first cluster is bounded from above and below by some given constants.

This problem has been studied only without additional constraints earlier. The strong NP-hardness of the problem without additional constraints was shown in [1]. There have been presented some algorithmic results too (see, [2], [3] and references therein). Unfortunately, these results can not be applied for the considered problem that is important, in particular, in data analysis and data mining, when the data having in the hands is a time series.

In this paper, we have shown that the considered problem is the strongly NP-hard one and propose a polynomial-time 2-approximation algorithm for solving the problem.

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Finding Multiple Solutions to a Class of p-Laplace Problems Using Newton's Method

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Keywords. Saddle points; p-Laplacian; Newton's method; Finite element method.

Classical critical point theory and traditional numerical methods mainly concern about finding local extrema. The critical points which are not local extrema called saddle points, which appears as unstable local equilibria or transient excited states in physical systems. Due to the unstable nature of saddle points, it is very difficult to compute them numerically in a stable way. The classical minimax principle characterizes saddle points as solutions to the two-level global minimax problem which is not useful for numerical implementation. Yao and Zhou [2] establish a local minimax characterization of saddle points and developed a numerical minimax method to solve quasi-linear elliptic PDE with the p-Laplace operator.

The Local Minimax method is a gradient type method, provides the first-order accuracy. If the corresponding energy functional $J \in C^2(W_0^{1,p}(\Omega), \mathbb{R})$, it is quite obvious to use Newton's method to speed up the convergence. However, for $p \neq 2$, $W_0^{1,p}(\Omega)$ is not isomorphic to its dual $W^{-1,q}(\Omega)$, as a consequence any critical point of J is degenerate in the classical sense. Hence, Newton's method can not apply directly. Therefore, we use Morse theory for Banach space [1] to overcome this degeneracy problem. Then we have used Newton's method together with the finite element method to solve the p-Laplace problem numerically.

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An enhanced BASBL solver for bilevel problems

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Keywords. Bilevel programming; Global optimization; Optimization software; BASBL solver; BASBLib.

Bilevel programming problems (BPP) are a class of very challenging optimization problems arising in many important practical applications, including transportation, pricing mechanisms, airline and telecommunication industry, chemical and civil engineering, machine learning, etc. The numerous various applications of bilevel programming problems provide a strong incentive for developing efficient solvers for this large class of problems. While (BPP) has been studied for a long time, the currently available software codes are mainly limited to special subclasses.

To address this, we present the most recent implementation of the Branch-And-Sandwich BiLevel solver (BASBL) capable of handling very general (BPP) problems. The BASBL solver is implemented within the open-source MINOTAUR (`http://wiki.mcs.anl.gov/minotaur`) toolkit and is based on the deterministic global optimization Branch-and-Sandwich algorithm introduced in [1,2], and extended in [3]. The performance of BASBL has been investigated with a detailed numerical study using the bilevel test problems from BASBLib (`http://basblsolver.github.io/BASBLib/`), and problems derived from practical applications using various algorithmic options. The results demonstrate the promising performance of BASBL.

The further BASBL developments, along with the possible directions, are summarized at the end of the talk.

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Delay-dependent on Robust Exponential Stability Analysis and H_∞ Performance for Uncertain Neutral Time-varying Delays Systems

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Keywords. Exponential stability; H_∞ performance; Time-varying delay; Neutral system.

The delay-dependent problems on robust exponential stability and the H_∞ performance for the uncertain neutral systems with time-varying delays is focused in this paper. By constructing a suitable augmented Lyapunov-krasovskii functional with quadruple integral terms. Combined the integral inequalities and the free weight matrices techniques, some delay-dependent exponential stability criteria and a prescribed performance index of H_∞ performance are yielded inform linear matrix inequality(LMIs). The numerical examples are finally shown the efficiency of the proposes method over some previous literature.

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Epidemic spreading curing strategy over directed networks

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Keywords. Epidemic spreading; NIMFA model; directed networks; genetic algorithms.

The diffusion of viruses within networks or among people has always attracted a lot of attention in many different research fields such as computer science, physics, medicine, and biology. The development of policies to control the epidemic spreading is a crucial problem. Epidemic models represent the network subject to the virus spreading with a graph where nodes are the individuals and the edges the direction of the infection from an infected individual to a susceptible one. One of the most popular epidemic models is the *Susceptible-Infected-Susceptible* (SIS) where a node can be either in the *susceptible* state S, in which it can contract the infection, or the *infectious* state I, in which it is infected. It is assumed that an individual can be reinfected, thus repeating the transition states $S \rightarrow I \rightarrow S$ eventually forever. In general, when controlling the evolution of epidemics, the network resources are limited. Thus, a challenging problem is the research of an optimal curing policy able to suppress the epidemic. In [1], we proposed a constrained Genetic Algorithm's based method to find a minimal-cost curing strategy over a weighted and directed network able to suppress the epidemic spreading by exploiting the *N-Intertwined Mean-Field Approximation* ($NIMFA$) of the SIS spreading process, introduced by [2]. Specifically, we focused on a heterogeneous setting where each node has its own curing rate and cost, and each node infects the other with a particular infection rate.

In this paper we consider the formulation of the optimization problem for directed weighted networks and extend the GA method to deal with not symmetric adjacency matrices that are diagonally symmetrizable.

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The singular value decomposition of the operator of the dynamic ray transform acting on 2D vector fields

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Keywords. Dynamic ray transform; singular value decomposition; vector field.

An inverse problem is called dynamic if the investigated object changes during the measuring process. Most reconstruction methods are based on the supposition that the object is static during the data collection. Therefore, an application of standard techniques in the dynamic case causes serious motion artefacts in the reconstructed image. So novel method in the case must take into account the constant changes of the object.

The position of the x-ray source is described by unit vector $\theta = (\cos(t\phi), \sin(t\phi))^T \in S^1$, which can be uniquely described by a time instance t and the rotation angel of the source ϕ. Also we consider dynamic setting with two-dimensional affine deformations. [1]

To construct singular value decomposition of the dynamic ray transform operator it is needed to choose an orthonormal system of vector fields in the initial space. For this aim we suggest to use harmonic and Jacobi polynomials. It is shown, that corresponding system of functions in the image space are constructed using harmonic and Gegenbauer polynomials. [2,3]

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Numerical investigation into a combined ecologically pure plasma-vortex generator of hydrogen and thermal energy

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Keywords. Swirling flow; numerical simulation; plasma-chemical reactions; plasma-vortex reactor.

One of the promising approaches in clean energy is hydrogen production using the hydration reaction of a metal micropowder, stimulated by plasma formations. The potential of that methodology, such as high thermal energy excess rates, hydrogen cost values close to the best world level, was demonstrated in [1]. However, industrial production of plasma-vortex reactors requires interdisciplinary optimization both mechanical and thermodynamic parameters of setup.

In present work, we carried out a series of numerical simulations of the turbulent three-dimensional swirling flow in plasma-vortex reactor to provide further insights into use of such apparatus. The modelling has demonstrated that desirable behavior with heat transferred mostly downstream can be ensured by use of pipe-like electrode placed downstream from cylindrical one. Pressure forces, occurring in such case, draw out the hot gas towards the exit nozzle. At the next step, we used exact experimental geometry and flow composition. Using optimized electrode system and simplified kinetic scheme of plasma-chemical reactions, we tested several operating modes of the PVR and obtained time dependent flow characteristics, which, in turn, will be used for further adjustment of the scheme and overall apparatus.

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A massively parallel Lipschitzian global optimizer

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Keywords. global optimization; high-performance computing; Lipschitz constant; performance comparison.

Lipschitzian global optimization is a promising and well-elaborated research area [1–5]. However, like any other deterministic global optimization techniques, it suffers from high computational complexity. Using high performance computing methods can significantly mitigate this issue. We propose an algorithm for massively parallel systems, e.g. many-core or GPU devices. The idea is to offload Lipschitzian constant estimation to a device and combine it with an incumbent value calculation. The estimation is done on a rectangular mesh making it highly suitable for massively parallel computations. We study the performance of the proposed approach on a number of benchmark problems and compare it with other state-of-the-art global optimization algorithms.

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Computer modeling of electrochemical impedance spectra for defected phospholipid membranes: finite element analysis

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Keywords. Finite element analysis; computer modeling; electrochemical impedance; phospholipid membranes.

Tethered bilayer lipid membranes (tBLM) are popular experimental platforms for studying protein-membrane interactions. One of alternating current (AC) techniques used to assess dielectric properties of such membranes is electrochemical impedance spectroscopy (EIS). While this method is useful for determining macroscopic properties of bilayers, it provides no direct information on structural properties of membranes containing defects. Such cases often require more complex microscopy techniques, such as atomic force microscopy (AFM).

The goal of this study was to investigate the relation between EIS spectral features and structural properties of defected membranes. We applied finite element analysis (FEA) technique to model EIS spectra for various defect distributions [1]. Three-dimensional membrane models were implemented and solved with COMSOL Multiphysics FEA software.

Both experimentally registered by AFM and computer-generated defect distributions of varying density and defect size were used in modeling. Comparison of modeled EIS spectra for heterogeneous defect distributions and analytical EIS solutions of homogeneous distributions indicated only quantitative differences between the two approaches. EIS spectra modeled with experimentally registered defects and computer-generated distributions of equivalent density exhibited discrepancies in cases of defect clusters present in experimental data. Comparing experimentally measured EIS spectra of real membranes with modeled spectra revealed significant correlation between EIS spectral features of both datasets.

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Improved less conservative stability criteria for stochastic uncertain discrete-time neural networks with mixed delays and an impulse

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Keywords. Stochastic discrete-time recurrent neural networks; Leakage time varying delays; Lyapunov-Krasovskii functional; Global asymptotic stability; Impulses.

In this paper, we deal with the stability analysis problem for stochastic impulsive discrete-time recurrent neural networks with both time-varying discrete delays and time-varying leakage delays. By utilizing the linear matrix inequality method, stochastic analysis approach and a well-known inequality of Jenson, a new Lyapunov-Krasovskii functional is constructed to derive the global exponential stability in the mean square for the addressed recurrent neural networks with stochastic perturbations and impulsive disturbance. Moreover, the results are compared with some existing works in the literature and it shows the less conservatives of our system. The derived exponential stability criteria are made dependent on both the time-varying delays and the leakage delays, and are therefore it is less conservative than the delay independent criteria of traditional discrete-time neural network model. In addition to that, numerical examples with computer simulations are presented to illustrate the usefulness and effectiveness of the proposed theoretical results.

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A system of p-Laplacian equations on the Sierpiński gasket

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Keywords. Sierpinski gasket; p-Laplacian; weak solutions; p-energy; system of equations.

Differential equations on fractals is an active area of research for the past few decades. Problems on fractal domains lead to nonlinear models, for example, reaction-diffusion equations, problems on elastic fractal media or fluid flow through fractal regions. Earlier many researchers have studied Laplacian equations on fractal domains, but there is not much literature on p-Laplacian equations on fractals due to some difficulties in handling these equations. So, we are interested in studying p-Laplacian equations on fractals.

We have studied following system of equations on the Sierpiński gasket.

$$\begin{aligned} -\Delta_p u &= \lambda a(x)|u|^{q-2}u + \frac{\alpha}{\alpha+\beta}h(x)|u|^{\alpha-2}u|v|^{\beta} \text{ in } \mathcal{S}\setminus\mathcal{S}_0; \\ -\Delta_p v &= \gamma b(x)|v|^{q-2}v + \frac{\beta}{\alpha+\beta}h(x)|u|^{\alpha}|v|^{\beta-2}v \text{ in } \mathcal{S}\setminus\mathcal{S}_0; \\ u &= v = 0 \text{ on } \mathcal{S}_0, \end{aligned} \tag{1}$$

where $\mathcal{S}$ is the Sierpiński gasket in $\mathbb{R}^2$, $\mathcal{S}_0$ is the boundary of $\mathcal{S}$ and Δ_p denotes the p-Laplacian where $p > 1$.

We have proved the existence of two nontrivial weak solutions of problem (1) under suitable conditions on parameters involved in the equations. We have used Nehari manifold and fibering map like technique to the show existence of solutions.

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Performance comparison of a geophysical code on manycore processors and hybrid clusters

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Keywords. Elastic wave; manycore systems; finite difference scheme; HPC; GPU; vectorization.

The solution of actual numerical simulation problems requires the development of parallel programs that efficiently use modern computational architectures. There is a possibility of choosing not only various mathematical methods and algorithms for solving a problem, but also various computational architectures. Therefore researchers have to solve a difficult task of determining the optimality of such a choice, which is often solved on partially intuitive level [1].

In this paper, the problem of seismic wave propagation in elastic 3D media typical of magmatic volcanoes is considered [2]. Using a finite difference method to solve this problem as an example, the features of the development and optimization of parallel codes for various modern multi-core architectures (Intel Broadwell, Intel Knights Landing, IBM POWER9, NVIDIA Fermi, NVIDIA Kepler) are considered. The effect of various strategies of computations and memory optimization on the final performance is investigated. We consider specific optimizations for different types of architectures.

Based on the carried out research, a high-performance software has been developed for the three types of clusters: equipped with processors Intel Xeon, Intel Xeon Phi and graphics accelerators. High scalability scores have been achieved.

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Analysis of systems for operational data processing based on Big Data and their practical application

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Keywords. improve routing; air pollution; Neural network .

This article proposes a solution to improve routing and tracking the status of heterogeneous cargo to its destination, using GPS sensors and radio frequency identification (RFID) [1].

From large cargo emissions and air pollutants emissions, a solution is proposed, using IoT technologies, to collect incoming data on air humidity, temperature and maximum permissible concentrations of particulate matter in the atmosphere. Currently, all data is written manually in paper form and then transferred to a computer[2]. The authors analyze the existing systems and improve the existing ones.

The deterioration of environmental living conditions due to the large release of carbon dioxide into the environment leads to a decrease in the General condition of the human body and the development of cardiovascular diseases and cancer, tuberculosis, diabetes and others. According to the Universal health organization, cancer is in second place in mortality, both in the world and in Kazakhstan. It is recommended to build a neural network to identify the early stages of cancer of the citizens of the Republic of Kazakhstan, as well as General monitoring of the patient, forecasting the results of different methods of treatment and analysis of the effectiveness of the treatment.

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On an effective usage of numerical infinities and infinitesimals in economic models

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Keywords. Infinity in Economic Models; Infinity Computer; Numerical Computations; Paradoxes

There exist numerous economic models where infinite and infinitesimal quantities play an important role. It is sufficient to mention as examples infinite decision processes such as fair lotteries and other repeated games, games with an infinite number of players, and games appealing to infinitesimal probabilities. A typical example is the St. Petersburg paradox introduced by N. and D. Bernoulli in the early XVIII-th century. This paradox and other similar problems have attracted attention of numerous mathematicians and economists starting from De Morgan, Euler, Cournot, and Poisson, and more recently by Keynes, Arrow, Samuelson, Aumann, and Dutka. Unfortunately, traditional mathematical tools used to study these situations do not allow scientists to obtain unique, non disputable answers and often lead to very different results and paradoxes.

In our opinion, the reason is that traditional techniques either lead to various kinds of divergences and, as a consequence, become intractable mathematically or are based on purely symbolic considerations not involving numerical mathematics. In this talk, we discuss recent studies [1, 2] that approach infinite fair lotteries and some other infinite games numerically. This is done by applying a novel computational methodology (see [3, 4]) giving the possibility to execute calculations with infinite, finite, and infinitesimal floating-point numbers. All of them (including the infinite ones) can be effectively stored in the memory of the supercomputer [3] and treated numerically. Advantages of this new, essentially numerical point of view on old economic models are discussed in the talk.

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Practical Enhancements for the LP/NLP Algorithm for Convex MINLPs

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Keywords. Convex MINLP; LP/NLP algorithm; Valid inequalities.

The LP/NLP based branch and bound [1] is one of the most effective algorithms for solving convex mixed-integer nonlinear programs (MINLPs). The algorithm starts by creating a mixed-integer linear relaxation of the nonlinear feasible region which is in turn solved by means of branch-and-cut. The linear relaxation is created using gradient based linear approximation of the functions in the constraints or objective. More such inequalities are added in order to obtain tighter relaxations as the algorithm progresses. While the algorithm is known to take finite number of steps, careful implementation and control are required for it to be practically useful. Convex MINLPs are known to be $\mathcal{NP}-$hard, and this algorithm, like others, can take long time to run. We demonstrate effectiveness of some practical ideas that enhance the performance of this algorithm. These methods have been implemented in the open-source MINOTAUR optimization toolkit and tested on benchmark instances.

First, we describe methods to detect the appropriate conditions for adding more inequalities. Adding them only when we reach integer feasible points in branch-and-cut tree may lead to a weak relaxation and hence a large tree, and adding too many of these early on can slow down the solution time. We use the primal and dual information provided by the solution of each node of the tree and the existing inequalities to ascertain whether new inequalities should be generated. Next, we describe methods to generate tight inequalities. A tight inequality should ideally touch a face of feasible region and also cut off a large portion of the relaxation. When a nonlinear constraint has both a nonlinear and a linear function with different variables, finding such an inequality is relatively easy and does not require solving a nonlinear problem. We note that this particular structure is widespread: almost all convex instances in the MINLP Library [2] exhibit this property in at least one constraint. Third, we present line search based methods for finding good points for generating linear inequalities when this structure is missing.

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Developing clustering algorithm for descriptor entities in education sector

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Keywords.
descriptor approach; competence approach; semantic similarity.

The article proposes the algorithm to solve objects clustering problem for such subject areas as education and labour market. Such objects are competency, discipline, specialty, vacancy, etc. The main problem in clustering algorithm development proved to be the stage of attributes design since the named objects have descriptions in natural language. Consequently, a descriptive model for the objects was designed at first. The model was based on the fact that all necessary concepts are characterised in the space of descriptors "know", "can", etc. [1].

This allowed the object to be represented as a tuple based on the object name, descriptors (and their values) and keywords related to descriptors. To obtain such structures, the toolkit of context-relative text mining was used. The ability to represent the entities in question as a formal structure allowed the attribute space formation algorithm to be developed and complex metrics to be constructed to solve the stated clustering problem. The developed algorithm permits development of various services for a faster and more objective decision-making process in educational and professional sectors [2].

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Compact filter regularization and error estimate for solving sideways heat equation

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Keywords. Sideways heat equation; Compact filter regularization; Ill-posed problem; Error estimates.

In this paper, the sideways heat equation [1], sometimes referred to as the inverse heat conduction problem is considered to obtain a stable numerical solution. The sideways heat equation is a model of a problem where one wants to determine the temperature on both sides of a thick wall, but cannot measure the temperature on one side due to its inaccessibility. It is ill-posed in the sense of Hadamard, i.e., the solution (if it exists) does not depend continuously on the final temperature. Due to measurement and computational error, the numerical recovery of temperature at one end from measured data is a tough task. To overcome such difficulties, some regularization techniques [2, 3] are required.

In this paper, the stable approximate solution of the sideways heat equation is obtained numerically using a compact filter regularization [4]. Proposed fourth-order compact filtering is first time used here as a new regularization technique of sideways heat equation where filtering is done in space rather than a Fourier domain. The heat equation is discretized by a differential-difference equation, where the time derivative has been replaced by a finite difference, and we analyze the approximation properties of time-discrete approximations using Fourier techniques. An error estimate between the exact and regularized solution is derived. The step length in the time discretization plays the role of the regularization parameter. Numerical examples are given to show that the method works effectively.

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Finite Difference Approximation for Space-Time Fractional Diffusion Wave Equations

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Keywords. Implicit finite difference method; Riesz space-fractional derivative; Stability; Convergence.

The traditional wave equations are used to model the wave propagation in an ideal conducting medium. For characterizing the wave propagation in an inhomogeneous medium with frequency dependent power-law attenuation, the space time fractional diffusion wave equations (FDWEs) appears [1]. In these equations, the power law behavior is characterized by the fractional derivative. The range of the exponent of power-law varies from 0 to 2 for example, for most solid and highly viscous materials, it is close to 2, while for some medium of practical interest such as bio-materials, it is from 1 to 1.7. Some of the applications of FDWEs include charge transport in amorphous semiconductors [2], propogation of mechanical waves in visco-elastic media [3] and many more.

This paper is concerned with the space-time fractional diffusion wave equation having different space and time fractional order. We consider an implicit unconditional stable finite difference method for solving time-space fractional diffusion wave equations. We use the Gerschgorin theorem to study the stability and consistency of the method. We also find the analytic solution for the same. Numerical solution of the proposed fractional diffusion-wave equation is obtained and the behavior of the error is examined to verify the order of convergence.

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Artificial Neural Network Model to Prediction of Eutrophication and *Microcystis aeruginosa* Bloom in Maekuang Reservoir, Chiangmai, Thailand

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Keywords. Artificial Neural Network model; eutrophication; toxic cyanobacteria.

Maekuang reservoir is one of the water resources which provides water supply, livestock and recreational in Chiangmai city, Thailand. The water quality and *Microcystis aeruginosa* are a severe problem in many reservoirs. *Microcystis aeruginosa* is the most widespread toxic cyanobacteria in Thailand. Artificial Neural Network (ANN) model is a more powerful machine learning. ANN is able to learn from previous data and has been used to predict value. ANN consists of three layers as input, hidden, and output layer. Water quality data is collected biweekly at Maekuang reservoir (1999-2000). Input data for training including nutrients (ammonium, nitrate, phosphorus), Secchi depth, BOD, temperature, conductivity, pH and output data for testing as Chlorophyll *a* and *Microcystis aeruginosa* cells. Results indicate that the ANN can be predicted eutrophication indicators during the summer season and ANN has efficient for providing the new data set and predict the behavior of *Microcystis aeruginosa* bloom process.

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Acceleration of global search through dual Lipschitz constant estimates

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Keywords. Global optimization; multiextremal problems; Lipschitz constant estimates.

The paper considers global optimization problems with a black-box objective function satisfying the Lipschitz condition. Efficient algorithms for this class of problems require reliable estimates of the Lipschitz constant to be introduced. In fundamental work [1] various approaches have been proposed to take into account both global and local properties of the objective function. In particular, algorithms using local estimates of the Lipschitz constant have shown their potential [2, 3].

The new approach presented in this paper is based on simultaneous use of two estimates: one is substantially larger then the other. The larger estimate ensures global convergence and the smaller one reduces the total number of trials needed to find the global optimizer. Results of numerical experiments on the random sample of multidimensional functions demonstrate the efficiency of the suggested approach.

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The method of approximate inverse in slice-by-slice vector tomography problems

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Keywords. vector tomography; ray transform; solenoidal vector field.

Let a vector field be given in a three-dimensional unit ball. It is require to find the field by its known values of the ray transform, which maps vector fields to functions on a manifold of oriented lines.

The operator of ray transform has not trivial kernel. The kernel consists of potential vector fields with potentials that equal to zero on the unit sphere. Consequently we can reconstruct only solenoidal parts of vector fields from the ray transform.

In [1], [2] an algorithm of solving the problem of reconstruction of a solenoidal part of vector field was based on the inversion formulas [3]. The problem of recovering a solenoidal part of a three-dimensional vector field from ray transform known over all lines parallel to one of the coordinate planes was considered.

In this report we suggest an algorithm of solving the problem with the same scheme of data collection. The algorithm is based on the method of approximate inverse, which was successfully used to solve problems of two-dimensional vector and 2-tensor tomography [4].

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A Numerical Approach of a Certain Type of Mixed Functional Differential Equations

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Keywords. Mixed-type functional differential equations; numerical approximation; homotopy analysis method.

In applied sciences, a wide number of mathematical models show up functional differential equations with delayed and advanced arguments, the mixed type functional differential equations (MTFDEs). MTFDEs appear in applied sciences such as biology, quantum physics, economy, control, acoustics, aerospace engineering. Some recent numerical methods to approximate the solution of a linear MTFDE were introduced in [1] and improved in [2, 3]. More recently, these methods were adapted and used to solve numerically a nonlinear MTFDE [4]. This paper provides a technique to solve a functional nonlinear mixed differential equation. The proposed technique is based on homotopy analysis method. We analyze the performance and accuracy of the proposed method and compare with the results obtained previously using other numerical methods.

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Robust H_∞ control for polytopic uncertainties discrete-time neural networks with leakage time-varying delay

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Keywords. Discrete-time; Robust H_∞ control; Leakage time-varying delay; Polytopic uncertainties.

This paper is related to the robust H_∞ control problem for discrete-time neural networks (DNNs). The system with polytopic uncertainties, time-varying delay and time-varying delay of the leakage term is investigated. Our results are derived sufficient conditions in the form of linear matrix inequalities (LMIs). Base on the parameter dependent Lyapunov functional is presented to obtain delay dependent sufficient conditions for H_∞ optimal controller and S-procedure. The examples are given to show the effectiveness and guarantee of our theoretical results.

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Computational Fluid Dynamics Methods for Wind Resources Assesment

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Keywords. CFD; flow modelling; RANS equations; wind resources.

Increasing wind resource applicability leads to the interest of the wind turbine installations in areas with more uniform topography. In-site measurements could be the expensive and time-consuming way how to determine the suitability of the area for the wind power generation even there are used already existing infrastructures (such as telecommunications masts) for the mounting of measurement sensors. The alternative is to use numerical methods, for example, Computational Fluid Dynamics (CFD).

In this research, the typical topology near the Baltic Sea is analysed using Reynolds Averaged Navier-Stokes equations to evaluate numerically the turbulent airflow over coastal terrain. The multispectral satellite images are utilized to describe the topology of the interested area. Digital Elevation Model is used to generate the ground surface which is applied as the input to develop the high-resolution computational mesh of the coastal terrain. Computational domain parallelization and the computational cluster is applied due to the complexity of the numerical simulations. Obtained results are compared with experimentally measured data from wind speed sensors located on the telecommunication mast.

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On Stationary Points of Distance Depending Potentials

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Keywords. Coulomb potential; optimal facility location; Weber problem.

Given fixed points $\{P_j\}_{j=1}^K \subset \mathbf{R}^n, K \geq 3$ and the nonnegative reals $\{m_j\}_{j=1}^K$, we investigate the structure of the stationary point set for the function

$$F(X) = \sum_{j=1}^{K} m_j |XP_j|^L, \ X \in \mathbf{R}^n$$

with $|\cdot|$ standing for the Euclidean distance. We compare the structure of the stationary point sets for several values of the exponent $L \in \mathbf{R}$, focusing ourselves mainly onto the cases $n \in \{2, 3\}$ and

(a) $L = -1$, i.e. Coulomb potential for the point charges $\{m_j\}$ fixed at the positions $\{P_j\}$ [1];
(b) $L = +1$, i.e. the objective function for the Weber unifacility optimal location problem [2].

We develop the analytical approach to the problem aiming at finding the exact number of stationary points and their location in dependency of the parameters involved. Generalization of the problem to the case of the function

$$G(X_1, X_2) = \sum_{j=1}^{K} \left\{ m_{1,j}|X_1P_j|^L + m_{2,j}|X_2P_j|^L \right\} + m|X_1X_2|^L, \ \{X_1, X_2\} \subset \mathbf{R}^n$$

is also discussed.

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Learning Aerial Image Similarity using Triplet Networks

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Keywords. Image similarity; neural networks; localization.

Unmanned aerial vehicles (UAV) faces localization challenges in satellite navigation systems denied environments. Images taken from on-board cameras can be used to compare against orthophotographical map to support visual localization algorithms, such as particle filter localization, synchronous localization and mapping (SLAM). Image similarity estimation can be achieved calculating various similarity metrics, such as Pearson correlation, Mean squares, Pattern intensity or Mutual information. Pearson correlation is not robust against image displacement caused by aircraft frame movement, previous work [1] show that aircraft heading angle error of 5 degrees causes 35% decreased in correlation measure compared with matched image with no rotational error. In other hand, distance–based metrics (e.g. Mean squares) struggle from Curse of dimensionality. We propose a new architecture of triplet neuron network [2] to learn image similarity measure and to deal with such problems. The proposed architecture incorporates VGG16 network base layers, top layer structure being suggested by authors. Flight simulator was used to generate aerial images simulating UAV flight conditions. Images were matched to the maps from satellite photo. The matching results from proposed neural network architecture are compared and evaluated against Pearson correlation.

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Integral and differential operators as the tools of integral geometry and tomography

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Keywords. Integral operators; tensor tomography; integral geometry; ray transform; angular moment.

Integral and differential operators are important tools at settings, investigations and solving methods for problems of integral geometry, tensor and refraction tomography. Integral transforms represent the essence of tomography approaches, consisting in nondestructive mode of obtaining information, which is accumulated along lines of integration. At present a list of integral operators, describing initial data, is very vast. It includes such operators as generalized Radon transforms, weighted longitudinal, transverse and mixed ray transforms of tensor fields [1]-[3].

Second family of integral operators is applied for investigations and solving the problems of integral geometry and refractive tensor tomography. It should be recalled that inversion formulas for the Radon transform contain integral operators of back-projection, Riesz potential, Fourier and Hilbert transforms. A generalization of back-projection operator provides the operators of angular moments for attenuated ray transforms of tensor fields, et al. Differential operators of tensor analysis and the operators of angular moments, present useful tools for investigation of integral geometry and tomography problems [3].

Properties of attenuated weighted ray transforms and angular moments of ray transforms for tensor fields are established. The differential equations for generalized ray transforms and their connections are investigated.

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Modelling population size using Horvitz-Thompson approach based on the Poisson Lindley distribution

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Keywords. Poisson-Lindley distribution; Zero-truncated distribution; Horvitz-Thompson estimators; Variance estimation.

Capture-recapture analysis is applied to estimate the number of population in ecology, biology, social science, medicine, linguistics and software engineering. The Poisson distribution is one of the simplest models for count data and appropriate for homogeneous population. On the other hand, it is found to underestimate the counts for overdispersed data. In this study, I have focused on the mixture of Poisson and Lindley distribution which can exhibit overdispersed count data and right long tail. Consequently, there are some individuals unobserved, the zero-truncated Poisson Lindley distribution is considered. The parameter of distribution can be estimated using the maximum likelihood estimation. In simulation studies, the Horvitz-thompson estimator is presented for modelling the population size. Point and interval estimation of the target population under the zero-truncated Poisson Lindley distribution are proposed. The variance estimation by conditioning is used for the confidence interval of population size. Bias and mean square error are used for measuring the accuracy of the estimator. The simulation results show that the Horvitz-Thompson estimator under the zero-tuncated Poisson Lindley distribution provides a good fit rather than the zero-truncated Poisson distribution.

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On unconstrained optimization problems solved using CDT and triality theory

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Keywords. Canonical duality theory; extended Lagrangian, dual function.

D.Y. Gao solely or in collaboration applied his Canonical duality theory (CDT) for solving a class of unconstrained optimization problems, getting the so-called “triality theorems”.

As mentioned in the recent book [2], “triality theory can be used to identify both global and local optimality conditions and to develop powerful algorithms for solving challenging problems in complex systems”.

Unfortunately, the “double-min duality” from the triality theorems published before 2010 revealed to be false, even if in the paper [1] DY Gao announced that “certain additional conditions” are needed for getting it.

Beginning with 2011, D.Y. Gao together with some of his collaborators published several papers in which they added additional conditions for getting “double-min” and “double-max” dualities in the triality theorems; a general case is considered in [3], while particular cases are treated in several papers.

Our aim in this talk is to indicate an approach for treating rigorously this kind of problems and to discuss several results concerning the “triality theory” obtained up to now.

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Potential usefulness of the grossone and infinity computer in probability

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Keywords. probability theory; uniform distribution; binomial distribution; normal distribution

As comprehensively surveyed in [1], a recently developed grossone-based methodology is finding more and more potential applications in diverse areas. So far, all these applications were concentrated around such areas as linear algebra, computational mathematics and optimization. In this talk, we discuss different aspects of applied probability theory where this methodology could also be useful. Grossone, denoted by ①, can either appear as a version of infinity or in the form 1/, where it would signify an infinitesimal. Both appearances can be very handy. For example, we can think of the binomial distribution Bin(①,p), where ① is the number of Bernoulli trials and p is the probability of success in these trials. CLT (Central limit theorem) can be stated as saying that the distribution $[\mathrm{Bin}(①,p)-p①]/\sqrt{①}$ is approximately $N(0,1)$, Gaussian distribution with mean 0 and variance 1. As will be discussed in the talk, dealing with $[\mathrm{Bin}(①,p)-p①]/\sqrt{①}$, rather than with $N(0,1)$, may have some advantages. In particular, the set of values, where the distribution $[\mathrm{Bin}(①,p)-p①]/\sqrt{①}$ is supported, is clearly defined and hence when we will be manipulating with the limiting distribution we can always track its support and, for example, avoid assigning negative values for estimators of p.

The second appearance of ①, in the form 1/①, can be even more useful. Consider, for example, a standard uniform distribution on $[0,1]$ and its discretized version, the distribution assigning weights 1/(①-1) to points $i/①$ for $i = 1, 2, \ldots, ① - 1$ and weights 1/2① to points 0 and 1. Dealing with the discretized version allows us to avoid 'zero measure' discussions and makes interpretations of at least some results more intuitively clear. We shall discuss the problem of transforming discretized random variables and computing expectation of these random variable in detail. To a large extent, the discussions follow the lines used in studying 'computer arithmetic'; see [2].

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On some challenges in Bayesian global optimization

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Keywords. global optimization; Bayesian approach; statistical models.

Interest in Bayesian global optimization methods is increasing as well as in their applications. Despite the increasing interest, some crucial problems remain outside of the focus of researchers. A methodology of the selection of an appropriate statistical model of an aimed objective function is not available. Moreover, the estimability of parameters of some popular statistical models is questionable [1]. The majority of methods are based on the optimization of surrogate functions which are defined combining conditional mean and variance of a chosen statistical model without decision theoretic substantiation. Thus the contemporary developments seem moving away from the original ides to develop global optimization methods based on the theory of rational decision making under uncertainty. We argue for the continuation of the original concept of the Bayesian approach to global optimization. In the present paper we discuss the bi-objective selection of a current iteration of a global search method in the context of the theory of rational decision making under uncertainty. We show that some known methods are particular cases of the method of bi-objective selection. The appropriateness of a statistical model of a considered objective function during the optimization process is discussed. The possibilities of on old idea [2] of application of a dual model of an objective function for the development of hybrid algorithms are considered.

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Ranking-based Discrete Optimization Algorithm for Asymmetric Competitive Facility Location

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Keywords. Asymmetric Facility Location; Binary Choice Rule; Combinatorial Optimization; Random Search.

A competitive facility location is important for firms which provide goods or services to customers in a certain geographical area and compete for the market share with other firms. There are various facility location models and strategies to solve them, which differ by their ingredients such as a facility attraction function, customers behavior rules, decision variables, a search space, objective function(s), etc.

We address a discrete competitive facility location problem for an entering firm, which wants to locate some new facilities with fixed qualities in a geographical region, where similar facilities of other competing firms are already present. The problem contains an asymmetric objective function and uses a binary customers choice rule. Both an integer linear programming formulation and a heuristic optimization algorithm based on ranking of candidate locations are designed to solve the problem. The proposed algorithm is specially adopted for the discrete facility location problems by utilizing their features such as geographical distances and the maximal possible utility of candidate locations, which can be evaluated in advance. Performance of the algorithm was experimentally investigated by solving different instances of the discrete competitive facility location problem with an asymmetric objective function.

The results of the experimental investigation demonstrate that the proposed heuristic algorithm is able to determine the optimal solution for different instances of facility location problems, and notably outperforms well-known heuristic algorithm, which is considered as a good strategy for such kind of problems.

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Formulation of the preparation problem of a commercial product batch under uncertainty

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Keywords. Oil refining; mathematical tools of automated systems; production processes optimization; interval optimization.

Oil refining is a key industry of the world economy. The increasing production cost of hydrocarbons and global competition in the oil market contribute to stimulate the oil refining industry to optimize production scheme. The evolution of mathematical support of automated enterprise management systems is closely connected with the systems development at each level of management. And that mathematical tools performed from lower level to top level and invertedly by priorities [1].

Mathematical models of enterprise organizational and economic management and models of process control are widely presented in the literature and implemented in the information systems of enterprise. Operational-scheduled and dispatching production management one of the most complex problems. And operational planning of continuous production is not fully described in the literature and has no "box" solutions [2].

The paper deals with the blending problem of components from tanks to obtain the necessary quantity and quality of petroleum products in the product tank. The feature of the mathematical models is constructed under the constraint that the only quality indicators is specified. Interval and stochastic approaches are formalized to obtained uncertainty.

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