University of Calabria, Rende (CS), Italy
in cooperation with
Society for Industrial and Applied Mathematics, USA

Book of Abstracts
of the 2nd International Conference
and Summer School

Numerical Computations: Theory and Algorithms

edited by
Yaroslav D. Sergeyev
Dmitri E. Kvasov
Francesco Dell'Accio
Marat S. Mukhametzhanov

Pizzo Calabro, Italy
19–25 June 2016
http://wwwinfo.deis.unical.it/~yaro/numta2016

SCIENTIFIC COMMITTEE

Lidia Aceto, Italy
Andrew Adamatzky, UK
Yanqin Bai, China
Roberto Battiti, Italy
Luigi Brugnano, Italy
Oleg Burdakov, Sweden
Sergiy Butenko, USA
Sonia Cafieri, France
Cristian Calude, New Zealand
Domingos Cardoso, Portugal
Marco Cococcioni, Italy
Salvatore Cuomo, Italy
Louis D'Alotto, USA
Oleg Davydov, Germany
Renato De Leone, Italy
Francesco Dell'Accio, Italy
Alessandra De Rossi, Italy
Branko Dragovich, Serbia
Adil Erzin, Russia
Yury Evtushenko, Russia
Şerife Faydaoğlu, Turkey Elisa
Francomano, Italy
David Yang Gao, Australia
Manlio Gaudioso, Italy
Victor Gergel, Russia
Franco Giannessi, Italy
Tadepalli Gopal, India
Vladimir Grishagin, Russia
Peter Gritzmann, Germany
Mario Guarracino, Italy
Nicola Guglielmi, Italy
Vladimir Gurman, Russia
Jan Hesthaven, Switzerland
Xiaodong Hu, China
Luc Jaulin, France
Louis Kauffman, USA
Yuri Kochetov, Russia
Dmitri Kvasov, Italy
Hoai An Le Thi, France
Stefano Lucidi, Italy
Paolo Mancosu, USA
Maurice Margenstern, France
Francesca Mazzia, Italy
Nenad Mladenovic, France
Marco Panza, France
Massimo Pappalardo, Italy
Marcin Paprzycki, Poland
Panos Pardalos, USA
Hoang Xuan Phu, Vietnam
Raffaele Pisano, Australia
Yuri Popkov, Russia
Igor Pospelov, Russia
Oleg Prokopyev, USA
Davide Rizza, UK
Valeria Ruggiero, Italy
Maria Grazia Russo, Italy
Leonidas Sakalauskas, Lithuania
Yaroslav Sergeyev, Italy (**Chairman**)
Khodr Shamseddine, Canada
Theodore Simos, Greece
Andrea Sorbi, Italy
William Spataro, Italy
Rosa Maria Spitaleri, Italy
Alexander Strekalovsky, Russia
Roman Strongin, Russia
Gerardo Toraldo, Italy
Tatiana Tchemisova, Portugal
Hiroshi Umeo, Japan
Igor Volovich, Russia
Gerhard Wäscher, Germany
Gerhard-Wilhelm Weber, Turkey
Luca Zanni, Italy
Anatoly Zhigljavsky, UK
Antanas Žilinskas, Lithuania
Julius Žilinskas, Lithuania
Joseph Zyss, France

ORGANIZING COMMITTEE

Francesco Dell'Accio, Italy
(SIAM representative)
Adil Erzin, Russia
Vladimir Grishagin, Russia
Dmitri Kvasov, Italy
(**Chairman**)
Marat Mukhametzhanov, Italy
Clara Pizzuti, Italy
Yaroslav Sergeyev, Italy

Table of Contents

Numerical Computations: Theory and Algorithms
Second International Conference and Summer School

19–25 June 2016, Pizzo Calabro, Italy

Dear Participants,

Welcome to the Second International Conference and Summer School *NUMTA-2016* "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 NUMTA-2016 is organized in cooperation with the Society for Industrial and Applied Mathematics (SIAM), USA.

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

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

We are happy to inform you that researchers from the following 22 countries participate at the Conference: Australia, Canada, Croatia, Finland, France, Germany, Greece, Israel, Italy, Japan, Kazakhstan, Korea, Lithuania, Philippines, Portugal, Russia, Singapore, Sweden, Thailand, Turkey, UK, and USA.

Authors of selected talks will be invited to submit full papers to a special issue of the international journal *Applied Mathematics and Computation* produced by Elsevier and dedicated to the Conference.

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

- 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);
- International Association “Friends of the University of Calabria” (Italy);
- 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.

Yaroslav D. Sergeyev
Distinguished Professor
Chairman of NUMTA-2016

Plenary Lectures

Recent advances in the numerical solution of Hamiltonian PDEs

Luigi Brugnano, Felice Iavernaro

University of Firenze, Dipartimento di Matematica e Informatica "U.Dini", Italy
University of Bari, Dipartimento di Matematica, Italy
luigi.brugnano@unifi.it, felice.iavernaro@unifi.it

Keywords. Hamiltonian problems, Hamiltonian partial differential equations, Energy-conserving methods, Hamiltonian Boundary Value Methods, HBVMs.

The numerical solution of Hamiltonian and, more generally, conservative problems has been the subject of many researches in the last decades, resulting in the definition of the so called *Geometric Integration*, which is focused on the study of methods able to inherit important *geometrical properties* from the continuous dynamical system.

Concerning Hamiltonian problems, a natural feature to retain in the numerical solution is the conservation of the Hamiltonian (often referred to as the *energy*). In this respect, the extensively researched *symplectic* methods are generally able to approximately conserve the Hamiltonian function over exponentially long times, but under special assumptions. A relatively more recent approach consists in the definition of *energy-conserving* methods. In particular, a class of energy-conserving Runge-Kutta methods, named *Hamiltonian Boundary Value Methods (HBVMs)*, has been defined in the last few years [1, 2].

It is possible to extend the approach which such methods rely on, in order to cope with *Hamiltonian partial differential equations*, after a proper space semi-discretization. In this talk, we review the main facts concerning HBVMs and their use for solving Hamiltonian PDEs, with particular emphasis on the semilinear wave equation [1, 3] and the nonlinear Schrödinger equation [4].

References

[1] L. Brugnano, F. Iavernaro. *Line Integral Methods for Conservative Problems*. CRC Press, Boca Raton (FL), 2016.

[2] L. Brugnano, F. Iavernaro, D. Trigiante. A simple framework for the derivation and analysis of effective one-step methods for ODEs. *Applied Mathematics and Computation* **218** (2012) 8475–8485.

[3] L. Brugnano, G. Frasca Caccia, F. Iavernaro. Energy conservation issues in the numerical solution of the semilinear wave equation. *Applied Mathematics and Computation* **270** (2015) 842–870.

[4] L. Barletti, L. Brugnano, F. Iavernaro. *Work in progress*.

Classifying Cellular Automata Using Grossone

Louis D'Alotto

Department of Mathematics and Computer Science
York College/City University of New York
Jamaica, New York 11451 ldalotto@gc.cuny.edu

Keywords. Cellular Automata, Grossone, Dynamical Systems, Classification.

Cellular automata, originally developed by von Neuman and Ulam in the 1940's to model biological systems, are discrete dynamical systems that are known for their strong modeling and self-organizational properties. As with all dynamical systems, it is important to study and classify their long term behavior. The the original concept of classifying cellular automata was initiated by Stephen Wolfram in the early 1980's, see [3] and [4]. A later, more rigorous, measure theoretic classification scheme for one-dimensional cellular automata, see [1], was developed by Robert Gilman. However, owing to the fact that measure theory does not discriminate between countably infinite and uncountable (in the Cantor sense) sets, in this paper a new classification approach, based on the Infinite Unit Axiom and Grossone, see [2], is presented and shown that it builds a dynamical classification similar, and in some sense finer, to that of Gilman and Wolfram. The classification is also extended to the two-dimensional case (not considered by Wolfram or Gilman). Given a finite alphabet S, the domain space of one-dimensional cellular automata is the space of all bi-infinite sequences with elements taken from the alphabet S, in the two-dimensional case, the domain space is the space of all infinite configurations in the plane. Traditionally, these spaces are considered uncountable. However, by applying the Infinite Unit Axiom and Grossone, we could put an upper bound on the number of elements in these spaces. Hence the forward dynamics of different cellular automaton rules are studied and classified by actually counting (representing) the number of bi-infinite sequences (or configurations) that stay close, upon forward evolution, to a given initial sequence (configuration).

References

[1] Gilman, R., Classes of Linear Automata, *Ergodic Theory and Dynamical Systems*, 7, (1987) 105-118.
[2] Sergeyev, Ya. D., *Arithmetic of Infinity*, Edizioni Orizzonti Meridionali, Italy, 2003.
[3] Wolfram, S., Statistical Mechanics of Cellular Automata, *Reviews of Modern Physics*, Vol. 55, No. 3, (1983) 601-644.
[4] Wolfram, S., *A New Kind of Science*, Wolfram Media, Inc., IL, 2002.

Nonlinear programming and ①: algorithms

Renato De Leone

Università di Camerino, School of Science and Tehnology, Camerino (MC), ITALY
renato.deleone@unicam.it

Keywords. Nonlinear Programming, Algorithms, Exact Penalty Methods.

In [1] applications in Mathematical Programming have been presented of the novel approach to infinite and infinitesimal numbers proposed by Sergeyev in a book and in a series of papers [2, 3, 4]. In particular, it has been shown that the use of ① leads to de definition of a new differentiable exact penalty functions. Moreover, the relationship between stationary points of this penalty function and KKT points for the original Nonlinear Programming problem have been studied as well as the importance of (modified) Constrained Qualification CQ conditions.

In this talk we will discuss some algorithms, modifications of standard algorithms in nonlinear optimization, that are suitable for solving the unconstrained minimization arising from the penalization via ① of the nonlinear constrained problem.

Acknowledgements.

This research was partly supported by a GNCS-INdAM 2014 (Grant Metodi Numerici per lottimizzazione non lineare).

References

[1] De Cosmis, S. and De Leone, R. (2012) *The use of Grossone in Mathematical Programming and Operations Research*, Applied Mathematics and Computation, 218(16), 8029-8038.

[2] Yaroslav D. Sergeyev. *Arithmetic of Infinity.* Edizioni Orizzonti Meridionali, CS, 2003.

[3] Yaroslav D. Sergeyev. A new applied approach for executing computations with infinite and infinitesimal quantities. *Informatica*, 19(4):567–596, 2008.

[4] Yaroslav D. Sergeyev. Numerical point of view on calculus for functions assuming finite, infinite, and infinitesimal values over finite, infinite, and infinitesimal domains. *Nonlinear Analysis Series A: Theory,Methods & Applications*, 71(12):e1688e1707, 2009.

A Unifying Theory and Deterministic Algorithm for Dealing with Challenging and "NP-Hard" Problems in Multidisciplinary Fields

David Y. Gao

Alex Rubinov Professor of Mathematics, Federation University Australia
d.gao@federation.edu.au

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

Duality is a beautiful, fundamental, and inspiring concept that underlies all natural phenomena. According to Sir M.F. Atiyah, duality in mathematics is not a theorem, but a principle. Therefore, duality gap is not allowed. For convex systems, mathematical theory of duality has been well-developed with extensive applications in engineering and sciences. However, in nonconvex and discrete systems, the classical Lagrange multiplier method and Fenchel-Moreau dualities suffer for producing different duality gaps. It turns out that many nonconvex variational/optimization problems are considered to be NP-hard.

Canonical duality theory is a breakthrough methodological theory, which can be used not only to model complicated phenomena within a unified framework, but also for solving a wide class of nonconvex/nonsmooth/discrete problems in multidisciplinary fields [1,2,3]. The associated triality theory reveals an interesting multi-scale duality pattern in complex systems, which can be used to identify both global and local extrema and to design powerful algorithms for solving challenging problems.

In this lecture, the speaker will first present a unified model for multi-scale complex systems, which lays a foundation for understanding complicated phenomena in nature, including bifurcation, chaos, game theory, information technology, logistics, manufactures, phase transitions, scheduling, and decision science, etc. Based on this model, he will show how a precise mathematical theory of duality was developed and why this theory can be used for dealing with not only the most challenging problems in nonlinear sciences, such as the chaotic dynamics and post-buckling of structures, but also a large class of so-called NP-hard problems in operations research and computer science. The inner connection between this theory and other popular methodologies, such as SDP method in nonconvex/integer programming and HQ regularization in image process, will be discussed. Applications will be illustrated by some well-known benchmark problems in d.c. programming, sensor networks and bi-level topology optimization of structural design. A very interesting relation between chaos in nonlinear dynamics and NP-Hardness in global optimization will be revealed.

This talk will bring some fundamental new insights into nonconvex sciences, global optimization, complex systems, and computational mathematics.

References

[1] Gao, D.Y. (2000). *Duality Principles in Nonconvex Systems: Theory, Methods and Applications*. Springer, xviii+454pp.

[2] Vittorio Latorre, David Y. Gao (2015). *Global Optimal Trajectory in Chaos and NP-Hardness*.

[3] David Y Gao, Ning Ruan, Vittorio Latorre (2015). Canonical Duality-Triality Theory: Bridge Between Nonconvex Analysis/Mechanics and Global Optimization in Complex Systems. In *Canonical Duality-Triality: Unified Theory for Multidisciplinary Sciences*, Springer.

Generating Sparse Representations by Adaptive Multiscale Approximation

Angela Kunoth

University of Cologne, Germany
kunoth@math.uni-koeln.de

Keywords. Approximation, Computation on infinite structures, Emerging computational paradigms.

Facing the challenge to extract and represent information inherent in masses of data or in complex systems, adaptive approaches based on multiscale representations play an important role in current scientific research in many areas of science. The leading paradigm is to spend a minimal amount of degrees of freedom and work while extracting and representing the maximal amount of information. This approach allows one to principally work with computer platforms of any size since it is ultimately steered by the availability of a certain budget.

I want to discuss two classes of problems for which adaptive multilevel schemes can be developed along this line. The first class concerns explicitly given information and discusses the problem of fitting nonuniformly distributed data to approximate multivariate functions. The second class deals with approximating optimization problems for operator equations, specifically, control problems constrained by elliptic and parabolic partial differential equations which may, in addition, have stochastic coefficients. Here the information - the state and control of a system - is contained implicitly. Both applications have in common that the solution method is based on minimizing a quadratic functional and that the concept of adaptivity in a coarse-to-fine fashion plays a central role. For developing solution schemes of optimal complexity, I also address fast iterative solvers.

Computational Models and Challenging Global Optimization Problems

Panos M. Pardalos

University of Florida, USA
Higher School of Economics, Nizhny Novgorod, Russia
http://www.ise.ufl.edu/pardalos/, http://nnov.hse.ru/en/latna/

Keywords. Traditional and emerging computing models; intractable optimization problems; complexity; heuristics and their evaluation.

Most of the conventional computer models are based on the von Neumann computer architecture and the Turing machine model. However, quantum computers (several versions!), analog computers, dna computers, and several other exotic models have been proposed in an attempt to deal with intractable problems. We are going to give a brief overview of different computing models and discuss several classes of optimization problems that remain very difficult to solve. Such problems include graph problems, nonlinear assignment problems, and global optimization problems. We will start with a historical development and then we will address several complexity and computational issues. Then we are going to discuss heuristics and techniques for their evaluation.

On some computational issues in biology, ecology and population theory.

Ezio Venturino

Università di Torino, Dipartmento di Matematica "Giuseppe Peano", via Carlo Alberto 10, 10123 Torino, Italy
ezio.venturino@unito.it

Keywords. Predator-prey; genetic variability.

In this lecture a few recently introduced models in population theory will be presented, exploiting in some cases new ideas.

Group defense in predator-prey systems has been proposed in the current literature, but a different concept is represented by herd behavior. We will explore its consequences with an application to the case of the invasion of the European hare in Northern Italy. The novelty of this idea is also reflected in system dynamics that differs quite markedly from the classical quadratic models.

Herbivores grazing of tree barks represents a phenomenon with high potential impact on forests in natural parks, [3]. To study it, state-of-the-art approximation methods have been devised and will be outlined. These methods are also useful to assess the prevailing strain in the presence of two different diseases, [2].

Modeling disease propagation is a major task in epidemiology. We consider the case of a goat disease due to a lentivirus, and a way of fighting it. Mathematical modeling provides a new perspective for solving the problem. Genetic variability in interacting populations has also been considered and will be reviewed, discussing a few different instances in the demographic interactions, [4].

If time allows, we present also a very recent model for investigating diseases among the main insect pollinators, the bees, affected by mites, [1]. Also, a few examples will be illustrated of more complex models involving populations, partitioned by human artifacts or natural events, that start to evolve independently.

References

[1] Bernardi S., Venturino E. (2016) Viral epidemiology of the adult *Apis Mellifera* infested by the *Varroa destructor* mite, *Heliyon* Vol. 2 e00101, 43 pp. + 8 Appendix. http://dx.doi.org/10.1016/j.heliyon.2016.e00101

[2] Cavoretto R., Collino S., Giardino B., Venturino E. (2015) A two-strain ecoepidemic competition model, *Theoretical Ecology*, Vol. 8(1), pp. 37-52.

[3] Sabetta G., Perracchione E., Venturino E. (2015) Wild herbivores in forests: four case studies. In *Biomat 2014*, (edited by R. P. Mondaini), World Scientific (Singapore), pp. 55-77.

[4] Venturino E. (2012) An ecogenetic model, *Appl. Math. Letters* Vol. 25, pp. 1230-1233.

Classical areas of mathematics and statistics where the concept of grossone could be useful

Anatoly Zhigljavsky

Cardiff University and Lobachevsky Nizhny Novgorod State University,
Cardiff CF24 4AG, UK
ZhigljavskyAA@cardiff.ac.uk

Keywords. infinity, Grossone; divergent series; conditionally convergent series, infinity computer, improper prior

In this talk, I will consider several areas of mathematics where the notion of grossone developed by Ya. Sergeyev in his small book [1] and a series of papers, can be very useful. I will start with discussing the axioms of grossone and suggest some minor variations to the axioms of Ya. Sergeyev. The version of the grossone, which I will be using, will allow me to consider limits of divergent sequences.

Then I will mostly follow [2] and consider the summation of conditionally convergent and divergent series in the classical sense but using the notion of grossone. I will demonstrate that there are many situations where standard calculations can be made much easier and more convenient if grossone is adequately used. In particular, I will demonstrate that the sum of a conditionally convergent series $\sum_{n=1}^{\infty}$ is uniquely defined if the sign ∞ is replaced by the grossone. As a consequence, this sum does not depend on the rearrangement of terms and therefore the sum can be computed in many different ways. For example, it can be computed backwards rather than forward.

I will argue that the grossone can be very useful for analyzing methods of summation of divergent series. The use of grossone will allow me to introduce probability measures like the discrete uniform or binomial distributions on the set $\{1,2,\ldots,①\}$. This will allow me to give a probabilistic interpretation to many methods of summation of divergent series and hence compare their summability ranges.

Finally, I will consider the use of improper discrete priors in the Bayesian statistics and will argue, for example, that the use of the uniform improper prior on the infinite discrete set $\{1,2,\ldots,①\}$ can have a very clear interpretation. This can be of significance in biological applications, for example, when the parameter N of the binomial distribution $\mathrm{Bin}(N,p)$ is often assumed as having improper prior.

Acknowledgement. Research was supported by the Russian Science Foundation, project No. 15-11-30022 "Global optimization, supercomputing computations, and applications".

References

[1] Sergeyev, Y. D. (2013) *Arithmetic of infinity.*
[2] Zhigljavsky, A. (2012). Computing sums of conditionally convergent and divergent series using the concept of grossone. *Applied Mathematics and Computation,* 218(16), 8064-8076.

Global Search as a Sequence of Rational Decisions under Uncertainty

Antanas Žilinskas

Vilnius University, 4 Akademijos, Vilnius, LT-08663, Lithuania
antanas.zilinskas@mii.vu.lt

Keywords. Global optimization; decisions theory; kriging.

A review is presented on global optimization methods based on the principles of rational decision making under uncertainty. The considered methods are aimed at expensive black box objective functions. Optimization problems of that type are quite frequent in practical applications where objective functions are available as computer programs, and their properties are difficult to elicit. Uncertainty in the properties and expensiveness of objective function complicate the solution of the optimization problem. To substantiate a reasonable method for such problems we propose to appeal to the theory of rational decision making under uncertainty. The following themes are discussed in the talk:

- The selection of a statistical model of objective functions; the suitability of several stochastic functions for a model is discussed, possible generalizations are supposed.
- The postulates of a rational search strategy are formulated, and the corresponding algorithms are described.
- New ideas in axiomatic definition of a search strategy are discussed.
- The convergence and practical efficiency.
- The implementation problems.
- Generalization of the mentioned above ideas and results to the problems of multi-objective optimization.
- Visualization of Pareto optimal solutions/decisions.

New ideas are discussed as well as well known results, presented e.g. in [1, 2], are critically reconsidered.

Acknowledgements.

This work was supported by the Research Council of Lithuania under Grant No. MIP-051/2014.

References

[1] Torn A., Žilinskas A. (1989) *Global Optimization*. Springer, Berlin.
[2] Zhigljavsky A., Žilinskas A. (2008) *Stochastic Global Optimization*. Springer, New York.

Tutorials

The LION way: machine Learning for Intelligent OptimizatioN: a source of power for innovation in business

Roberto Battiti

DISI, University of Trento, Italy
Lobachevsky State University of Nizhny Novgorod, Russia
battiti@disi.unitn.it

Keywords. Machine learning, intelligent optimization, prescriptive analytics

Learning and Intelligent Optimization (LION) is the combination of machine learning from data and optimization to solve complex and dynamic problems. The LION way is about increasing the automation level and connecting data directly to decisions and actions. Prescriptive analytics is the third and final phase, beyond descriptive and predictive analytics. With support of the right software, more power is directly in the hands of decision makers in a self-service manner, without resorting to intermediate layers of data scientists.

In the tutorial we highlight the basic principles and mention some notable applications.

Acknowledgements.

The research in this tutorial was supported by the Russian Science Foundation, project no. 15–11–30022 "Global optimization, supercomputing computations, and applications."

Adoption of Unum Arithmetic: Two Approaches

John Gustafson

A*STAR, Singapore

john-gustafs@acrc.a-star.edu.sg

Keywords. Unum; Computer arithmetic;Energy-efficiency; Floating-point; Valid numerics; Computer simulation; Parallel processing; Interval arithmetic.

Unum arithmetic, introduced in early 2015, offers a long-needed advance in numerical computing over the IEEE floating-point types now in use. Unums eliminate rounding error, overflow, and underflow while using a limited number of bits. Rigorous bounds are obtainable without the overly pessimistic and loose estimates that result from the naive use of interval arithmetic methods. Energy and power consumption can be an order of magnitude less than floats, while producing better answers.

There are now two flavors of unums. One is upward compatible with IEEE floats, and can mimic them precisely to permit gradual replacement of floats with a better mathematical representation of a calculation. Three metadata fields are added to the IEEE format that permit numbers to be self-descriptive about their accuracy. The prototype environment, written in Mathematica, has been ported to Python, C, and Julia languages to make it fast and accessible. Processors with unum arithmetic in native hardware are being developed. This is one approach to making plausible the admittedly daunting task of evolving away from a century-old numeric format that is overdue for modernization. More recently, a second approach to unum arithmetic discards all compatibility with IEEE 754 Standard floats and constructs a mathematically airtight, elegant, concise, fast way to manipulate sets of real numbers with a numeric (non-symbolic) approach. These unums are of fixed size had have no redundant representations or wasted bit patterns. The idea of this approach is that floats and unums would coexist, just as floats and integers coexist in computing environments now, so that algorithms can gradually be converted to the new format. These unums have the remarkable property of being closed under reciprocation as well as negation, and all four basic arithmetic operations (plus, minus, times, divide) can finally execute with equal speed (a single clock cycle). Even the power function, x to the y power, can be executed in a single clock cycle, as can elementary functions such as logarithm, exponential, trig and inverse trig functions. Unums are able to solve problems that have defied solution by any other method to date.

The two approaches mirror what happened when parallel computing replaced serial computing, a revolution that is still underway; people could use gradual approaches such as shared memory and compiler directives, or they could choose between conventional serial computing and the more ambitious recoding needed to use message passing (MPI). Both approaches helped the community "boil the ocean" and make the switch. A similar two-pronged approach can help us restore mathematical validity to what has been a very approximate approach to handling real numbers for the last 60 years of electronic computing. After a brief introduction to the underlying concepts, examples of novel approaches physical simulations are given such as n-body dynamics, structural analysis, fluid dynamics, and other applications that show how unum computing not only provides provable bounds on computed predictions of behavior, but also can do it with massive data parallelism; we can easily find useful things to do with billion-core systems solving a single problem.

Episodes in the history of infinitesimals

Gabriele Lolli

Accademia delle Scienze di Torino, Italy
gabrielelolli42@gmail.com

Keywords. Infinitesimals; non archimedean fields; Cauchy; Cantor; Peano; Laugwitz; Sergeyev.

In [1] I gave a brief survey of the history of infinitesimals in mathematics. This time I will dwell on a few significant episodes of the modern tail of this history. In the nineteenth century Cauchy's original treatment was mistaken for a partial anticipation of Weierstrass and forgotten. Cantor's battle against du Bois-Reymond, Veronese et al. was taken as the end of infinitesimals. But only Peano came explicitely in support of Cantor, while Levi Civita in [2] already sowed the seeds of a new non metaphysical approach.

Towards the end of the twentieth century Laugwitz gave an algebraic simplification of non standard analysis, in [3] which can possibly also be a framework for Sergeyev's Grossone.

References

[1] G. Lolli, "Infinitesimals and infinites in the History of Mathematics: a Brief Survey", *Applied Mathematics and Computation*, vol. 218, issue 16, 2012, pp. 7977-8216.

[2] T. Levi-Civita, "Sugli infiniti ed infinitesimi attuali quali elementi analitici", *Atti Istituto Reale Veneto di Scienze, Lettere ed Arte*, ser. 7a, 4 (1892-1893), pp. 1765-1815.

[3] D. Laugwitz, "Ω-calculus as a generalization of field extension: An alternative approach to nonstandard analysis", in A. Hurd (ed.), Nonstandard analysis-recent developments, Springer, Berlin, 1983, pp. 120-133.

Numerical Computations with Infinities and Infinitesimals: Foundations and Applications

Yaroslav D. Sergeyev

University of Calabria, Via Pietro Bucci 42C, 87036 Rende (CS), Italy
Lobachevsky State University, Gagarin Av. 23, 603950 Nizhni Novgorod, Russia
yaro@dimes.unical.it

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

This tutorial presents a recently introduced (see [1–4]) methodology allowing one to execute numerical (not symbolic) computations with finite, infinite, and infinitesimal numbers in a unique framework. For this purpose a new type of supercomputer – the Infinity Computer patented in USA and EU – is used. This approach is based on the principle "The part is less than the whole" being Euclid Common Notion 5. The principle is applied to all numbers (finite, infinite, and infinitesimal) and to all sets and processes (finite and infinite). The methodology is not related to non-standard analysis and examines in detail the difference between mathematical tools used to describe mathematical objects and the objects themselves. In particular, it is stressed that numerals we use to write down numbers (finite, infinite, and infinitesimal) are among our tools and, as a result, they strongly influence our capabilities in studying numbers and other mathematical objects. Numerous examples and applications are given. The Infinity Calculator using the Infinity Computer technology is presented during the lecture.

Acknowledgements.

This work was supported by the project No. 15-11-30022 "Global optimization, supercomputing computations, and applications" of the Russian Science Foundation.

References

[1] Ya.D. Sergeyev. Lagrange Lecture: Methodology of numerical computations with infinities and infinitesimals. *Rendiconti del Seminario Matematico dell'Università e del Politecnico di Torino*, 68(2):95–113, 2010.

[2] Ya.D. Sergeyev. *Arithmetic of Infinity.* Edizioni Orizzonti Meridionali, CS, 2003, 2nd ed. 2013.

[3] Ya.D. Sergeyev. Un semplice modo per trattare le grandezze infinite ed infinitesime. *Matematica nella Società e nella Cultura: Rivista della Unione Matematica Italiana*, 8(1):111–147, 2015.

[4] Ya.D. Sergeyev. Computations with grossone-based infinities. *Unconventional Computation and Natural Computation: Proc. of the 14th International Conference UCNC 2015*, eds. Calude C.S., Dinneen M.J., LNCS 9252, Springer, New York, 89–106, 2015.

One-variable and Multi-variable Integral Calculus over the Levi-Civita Field and Applications

Khodr Shamseddine

University of Manitoba, Winnipeg, Canada
khodr.shamseddine@umanitoba.ca

Keywords. Levi-Civita Field; Non-Archimedean Analysis; Analytic Functions; Infinitesimals; Measure Theory and Integration; Double and Triple Integrals.

In this talk, we present a Lebesgue-like measure theory and integration on the Levi-Civita field $\mathcal{R}$. After reviewing the algebraic and order structures and basic elements of calculus on $\mathcal{R}$ [1], we introduce a measure that proves to be a natural generalization of the Lebesgue measure on the field of the real numbers and have similar properties. Then we introduce a family of simple functions from which we obtain a larger family of measurable functions and derive a simple characterization of such functions. We study the properties of measurable functions, we show how to integrate them over measurable sets of $\mathcal{R}$, and we show that the resulting integral satisfies similar properties to those of the Lebesgue integral of Real Analysis.

Then we generalize the one-dimensional measure and integration theory to two and three dimensions, showing that the resulting measures and double and triple integrals have similar properties to those from Real Analysis. Finally, we introduce so-called delta functions on $\mathcal{R}$, $\mathcal{R}^2$ and $\mathcal{R}^3$ which are piecewise analytic and integrable on the whole space with integral equal to 1 and which reduce to the Dirac delta function when restricted to real points; and we present simple applications of the theory.

References

[1] Shamseddine K. (2015) Analysis on the Levi-Civita Field and computational applications. *Journal of Applied Mathematics and Computation*, Vol. 255, pp. 44–57.

Special Sessions

Special Session

"Approximation Theory and Its Applications"

Organizers:

Maria Grazia Russo
University of Basilicata, Italy
Alessandra De Rossi
University of Turin, Italy

Towards efficient meshfree solvers

G.Ala[1], *E.Francomano*[2], *M.Paliaga*[2]

[1]University of Palermo, Scuola Politecnica, DEIM
[2]University of Palermo, Scuola Politecnica, DICGIM
guido.ala@unipa.it, elisa.francomano@unipa.it, marta.paliaga@unipa.it

Keywords. Meshfree methods; kernel functions; particle approximation.

In recent years meshfree methods have gained much attention in several application areas of science. These methods benefit of savings due to the elimination of the meshing process and are suited to handle changes in the geometry of the domain of interest. Further advantages come from the ease of implementation, which makes computer codes very flexible. We present some numerical experiences lying in the meshfree framework requiring function and its derivatives at nodes at scattered locations approximated by means of a kernel representation. Accuracy and computational efforts in modeling beyond the mesh are investigated. Numerical results are also discussed by referring to some test cases.

Acknowledgements.
This research was supported by INDAM-GNCS Project 2016.

References

[1] Ala G., Francomano E. (2015). Numerical Investigations of an Implicit Leapfrog Time-Domain Meshless Method. *Journal on Scientific Computing*, Vol. 62, pp 182–912.

[2] Ala G., Fasshauer G., Francomano E., Ganci S., McCourt M. (2015). The Method of Fundamental Solutions in Solving Coupled Boundary Value Problems for M/EEG. *SIAM J. Sci. Comput.*, Vol. 37(4), pp B570-B590.

[3] Fasshauer G.E. (2007). *Meshfree Approximation Methods with MATLAB*. World Scientific, Singapore.

[4] Liu G.R. (2009). *Meshfree Methods: Moving Beyond the Finite Element Method*. CRC Press.

Hermite-Birkhoff interpolation on arbitrarily distributed data on the sphere and other manifolds

Giampietro Allasia, Roberto Cavoretto, Alessandra De Rossi*

University of Torino, via Carlo Alberto 10, 10123 Torino, Italy
giampietro.allasia@unito.it, roberto.cavoretto@unito.it,
alessandra.derossi@unito.it

Keywords. Spherical approximation; Hermite-Birkhoff interpolation; Taylor expansions.

We consider the problem of interpolating a function given on scattered points using Hermite-Birkhoff formulas on the sphere and other manifolds. We express each proposed interpolant as a linear combination of basis functions, the combination coefficients being incomplete Taylor expansions of the interpolated function at the interpolation points [1, 4]. The basis functions have the following features: (i) depend on the geodesic distance; (ii) are orthonormal with respect to the point-evaluation functionals; and (iii) have all derivatives equal zero up to a certain order at the interpolation points. Moreover, the construction of such interpolants, which belong to the class of partition of unity methods [2, 3], takes advantage of not requiring any solution of linear systems. We give some numerical results in order to show the performance of the Hermite-Birkhoff interpolation.

References

[1] Allasia G., Bracco C. (2012) Multivariate Hermite-Birkhoff interpolation by a class of cardinal basis functions, *Appl. Math. Comput.*, Vol. 218, pp. 9248–9260.

[2] Cavoretto R., De Rossi A. (2012) Spherical interpolation using the partition of unity method: An efficient and flexible algorithm. *Appl. Math. Lett.*, Vol. 25, pp. 1251–1256.

[3] Cavoretto R., De Rossi A. (2014) A meshless interpolation algorithm using a cell-based searching procedure. *Comput. Math. Appl.*, Vol. 67, pp. 1024–1038.

[4] Wendland H. (2005) *Scattered data approximation*. Cambridge Monogr. Appl. Comput. Math., vol. 17, Cambridge Univ. Press, Cambridge.

RBF-PU interpolation with variable subdomain sizes and shape parameters

Roberto Cavoretto*, Alessandra De Rossi, Emma Perracchione

University of Torino, via Carlo Alberto 10, 10123 Torino, Italy
roberto.cavoretto@unito.it, alessandra.derossi@unito.it,
emma.perracchione@unito.it

Keywords. Meshfree approximation; RBF interpolation; Partition of unity methods.

The Partition of Unity (PU) method, performed with local Radial Basis Function (RBF) approximants, has been proved to be an effective tool for solving large scattered data interpolation problems [1, 2, 3]. But, in order to achieve a good accuracy, the question on how many points we can consider on each local subdomain, i.e. how large can be the local data sets, needs to be answered. Moreover, it is well-known that also the shape parameter affects the accuracy of the local approximants and, as a consequence, the one of the PU interpolant. Thus here, both the shape parameter used to fit the local problems and the size of the associated linear systems are supposed to vary among the subdomains. They are selected by minimizing an a priori error estimate. As evident from several applications provided, the proposed method turns out to be extremely accurate also when data with non-homogeneous density are considered.

References

[1] Cavoretto R., De Rossi A. (2015) A trivariate interpolation algorithm using a cube-partition searching procedure. *SIAM J. Sci. Comput.*, Vol. 37, pp. A1891–A1908.
[2] Cavoretto R., De Rossi A., Perracchione E. (2016) Efficient computation of partition of unity interpolants through a block-based searching technique. Submitted.
[3] Fasshauer G.E. (2007) *Meshfree approximation methods with* MATLAB, World Scientific, Singapore.

Two-points rational operators for univariate interpolation

Francesco Dell'Accio, Filomena Di Tommaso

University of Calabria, Via Pietro Bucci Cubo 30A, 87036 Rende (CS), Italy
francesco.dellaccio@unical.it, ditommaso@mat.unical.it

Keywords. Rational approximation; Multinode operators; Approximation order.

Two-points interpolation polynomials, such as Bernoulli, Lidstone and Hermite polynomials, have been combined with Shepard basis functions in order to improve the reproduction quality, and therefore the approximation order, of the classical Shepard method [1, 2, 3]. In this talk we propose to use those and others two-points polynomials in combination with recently introduced two-points rational basis functions. Some properties and the approximation order of the new combined operators are pointed out and compared with those given for classical combined Shepard operators.

Acknowledgements.
This research was supported by INDAM - GNCS Project 2016

References

[1] Caira R., Dell'Accio F. (2007) Shepard-Bernoulli operators. *Mathematics of Computation*, Vol. 76, pp. 299–321.

[2] Cătinaş T. (2003) The combined Shepard-Lidstone univariate operator. *Tiberiu Popoviciu Itinerant Seminar of Functional Equations, Approximation and Convexity*, Cluj-Napoca, May 21-25, 2003 , p. 3–15.

[3] Coman Gh. (1997) Hermite-type Shepard operators. *Rev. Anal. Numér. Théor. Approx.*, Vol. 26, pp. 33–38.

On the enhancement of the approximation order of the triangular Shepard method

Francesco Dell'Accio[1], Filomena Di Tommaso[1], Kai Hormann[2]

[1]University of Calabria, Via Pietro Bucci Cubo 30A, 87036 Rende (CS), Italy
[2]University of Lugano, Via Giuseppe Buffi, 6904 Lugano, Switzerland
francesco.dellaccio@unical.it, ditommaso@mat.unical.it,
kai.hormann@usi.ch

Keywords. Triangular Shepard method; Approximation order; Bernoulli polynomials.

Shepard's method is a well-known technique for interpolating large sets of scattered data. The classical Shepard operator reconstructs an unknown function as a normalized blend of the function values at the scattered points, using the inverse distances to the scattered points as weight functions. Based on the general idea of defining interpolants by convex combinations, Little [1] suggested extending the bivariate Shepard operator in two ways. On the one hand, he considers a triangulation of the scattered points and substitutes function values with linear polynomials which locally interpolate the given data at the vertices of each triangle. On the other hand, he modifies the classical point-based weight functions and defines, instead, a normalized blend of the locally interpolating polynomials with triangle-based weight functions which depend on the product of inverse distances to the three vertices of the corresponding triangle. The resulting triangular Shepard operator interpolates all data required for its definition, reproduces polynomials up to degree 1, whereas the classical Shepard operator reproduces only constants, and has quadratic approximation order [2]. In this talk we discuss on some improvement of the triangular Shepard operator. In particular, we substitute the linear polynomials with quadratic and cubic polynomials which approximate Bernoulli polynomials on the triangle in a least square sense and locally interpolate at the vertices. The resulting operators reproduce polynomials of degree greater than one and have approximation order greater than 2.

Acknowledgements.
This research was supported by INDAM - GNCS Project 2016

References

[1] Little F. (1983) Convex combination surfaces. In *R. E. Barnhill and W. Boehm, editors, Surfaces in Computer Aided Geometric Design*, North-Hollans p. 99–107.
[2] Dell'Accio F., Di Tommaso F., Hormann K. (2016) On the approximation order of triangular Shepard interpolation. *IMA Journal of Numerical Analysis* , Vol. 36, pp. 359–379.

On basins of attraction for a predator-prey model via meshless approximation

E.Francomano[1], *F.M.Hilker*[2], *M.Paliaga*[1], *E.Venturino*[3]

[1]University of Palermo, Scuola Politecnica, DICGIM
[2]Institute of Environmental Systems Research, Department of Mathematics and Computer Science, Osnabrueck, Germany
[3]University of Torino, Department of Mathematics G.Peano
elisa.francomano@unipa.it, frank.hilker@uni-osnabrueck.de, marta.paliaga@unipa.it, ezio.venturino@unito.it

Keywords. dynamical systems; predator-prey model; basins of attraction; meshless approximation.

In this work an epidemiological predator-prey model is studied. It analyses the spread of an infectious disease with frequency and vertical transmission within the predator population. In particular we consider social predators, i.e. they collaborate in group to hunt. The result is a three dimensional system in which predator population is divided into susceptible and infected.
Studying the dynamical system and the bifurcation diagrams it was identified a scenario in which the model can have a multistability. However the domain of attraction of one equilibrium point could be so small that it is almost the point itself. From a biological point of view it is very important analyses this effect to understand under which conditions the population go to the extinction or coexist.
Thus we present a study to analyse the basins of attraction of the stable equilibrium points. This paper addresses the research of the point lying on the surface which partitions the phase plane. Therefore a meshless approach has been adopted to give rise an approximation of the separatrix manifold.

References

[1] Alves M.T., Hilker F.M. (2014). Hunting Cooperation and Allee Effects in Predators. Preprinted submitted to *Journal of Theoretical Biology*.
[2] Cavoretto R., De Rossi A., Perracchione E., Venturino E. (2013). Reliable approximation of separatrix manifolds in competition models with safety niches. *International Journal of Computer Mathematics*, Vol. 92, No. 9, pp 1826–1837.
[3] Cavoretto R., Chaudhuri S., De Rossi A., Menduni E., Moretti F., Rodi M., Venturino E. (2011) Approximation of Dynamical System's Separatrix Curves. In Proceedings of the *AIP Conference 1389* (ed. by T.E. Simos et al.), Greece, pp 1220–1223.
[4] Fasshauer G.E. (2007) *Meshfree Approximation Methods with MATLAB*. World Scientific, Singapore.

Extended Lagrange interpolation in L^1 spaces

Donatella Occorsio, Maria Grazia Russo

University of Basilicata, Via dell'Ateneo Lucano 10, 85100 Potenza, Italy
donatella.occorsio@unibas.it, mariagrazia.russo@unibas.it

Keywords. Lagrange Interpolation; Polynomial Approximation; Product Quadrature Rules; Orthogonal Polynomials.

Let $w(x) = e^{-x}x^{\alpha}$, $\bar{w}(x) = xw(x)$ and denote by $\{p_m(w)\}_m, \{p_n(\bar{w})\}_n$ the corresponding sequences of orthonormal polynomials. $Q_{2m+1} = p_{m+1}(w)p_m(\bar{w})$ has simple zeros and the *Extended Lagrange Polynomial* $L_{m,m}(w, \bar{w}, f)$ interpolating a function f on the zeros of Q_{2m+1} can be considered. With $u(x) = e^{-\frac{x}{2}}x^{\gamma}$, $\gamma \geq 0$, let $C_u((0,+\infty))$ be the space of continuous functions f in any $[a,b] \subset (0,+\infty)$, equipped with the uniform norm. In this talk we will study the behavior of $\{L_{m,m}(w,\bar{w})\}_m$, being $L_{m,m}(w,\bar{w})$ a map from $C_u((0,+\infty))$ into suitable subspaces of $L^1_u((0,+\infty))$. This study completes the results given in [2], [1] in weighted $L^p_u((0,+\infty))$, for $1 < p \leq \infty$. As an application we show how to use the previous interpolation process in order to approximate weakly singular integrals

$$\int_0^{+\infty} f(x)K(x,y)w(x)dx = \int_0^{+\infty} L_{m,m}(w,\bar{w},f,x)K(x,y)w(x)dx + e_m(f,y)$$
$$:= \Sigma^*_{m,m}(f,y) + e_m(f,y).$$

Setting $\Sigma_m(f,y) = \int_0^{+\infty} L_m(w,f,x)K(x,y)w(x)dx$, it is more convenient to use $\{\Sigma_m(f), \Sigma^*_{m,m}(f)\}_m$ instead of $\{\Sigma_m(f)\}_m$, since we double the quadrature rule degree, by reusing m samples of f. This appears really relevant when m is "large". We prove the stability and the convergence of the quadrature rule, showing some numerical tests which confirm the theoretical estimates.

References

[1] Occorsio D. (2009) Extended Lagrange interpolation in weighted uniform norm, *Appl. Math. Comput.* Vol. 211 , no. 1, pp. 10-22.

[2] Occorsio D., Russo M.G. (2014) Mean convergence of an extended Lagrange interpolation process on $[0,+\infty)$, *Acta Math. Hungar.* Vol. 142 , no. 2, pp. 317-338.

Fast RBF OGr for Solving PDEs on Arbitrary Surfaces

Cécile Piret

Michigan Technological University, Mathematical Sciences, 1400 Townsend Drive, Houghton, MI 49931-1295
cmpiret@mtu.edu

Keywords. RBF; RBF-FD; OGr; Laplace-Beltrami.

The Radial Basis Functions Orthogonal Gradients method (RBF-OGr) was introduced in [1] to discretize differential operators defined on arbitrary manifolds defined only by a point cloud. We take advantage of the meshfree character of RBFs, which give us a high accuracy and the flexibility to represent complex geometries in any spatial dimension. A large limitation of the RBF-OGr method was its large computational complexity, which greatly restricted the size of the point cloud. In this paper, we apply the RBF-Finite Difference (RBF-FD) technique to the RBF-OGr method for building sparse differentiation matrices discretizing continuous differential operators such as the Laplace-Beltrami operator. This method can be applied to solving PDEs on arbitrary surfaces embedded in $\mathcal{R}^3$. We illustrate the accuracy of our new method by solving the heat equation on the unit sphere.

References

[1] Piret C. (2012) The orthogonal gradients method: A radial basis functions method for solving partial differential equations on arbitrary surfaces. *Journal of Computational Physics*, Vol. 231, pp. 4662–4675.

Introducing graded meshes in the numerical approximation of fractional differential problems

Magda Rebelo, Luísa Morgado

Centro de Matemática e Aplicações (CMA) and Departamento de Matemática, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, Quinta da Torre, 2829-516 Caparica, Portugal
Centro de Matemática, Pólo UTAD, Department of Mathematics, University of Trás-os-Montes e Alto Douro, UTAD, Quinta de Prados 5001-801, Vila Real, Portugal msjr@fct.unl.pt, luisam@utad.pt

Keywords. Fractional differential equation, Caputo derivative; Graded mesh.

One of the features in Fractional Calculus is that we cannot expect that the solution of a simple ordinary initial value problem, where the fractional derivative is given in the Caputo sense,

$$D^{\alpha}y(t) = f(t, y(t)), \quad y(0) = y_0,$$

to be smooth, even if the right-hand side function is smooth. A simple example is given by $y(t) = \dfrac{\sqrt{t}}{\Gamma(3/2)}$, which is the unique solution of the problem above with $\alpha = 1/2$, $f(t, y) = 1$ and $y_0 = 0$.
Since most of the numerical methods developed so far for this kind of problems assume certain regularity assumptions on the solution and the mesh used is uniform (that is, mesh with constant step size), in the cases where the solution is not as smooth as required, a decrease on the expected theoretical convergence order is usually observed. In order to overcome this, in this work we analyse and discuss the introduction of graded meshes in the approximation of Caputo derivatives of a function y which may be nonsmooth. These graded meshes are constructed through a graded exponent which is determined taking into account the type of singularity of y allowing us to obtain a mesh which is refined near the singular points.
Several illustrative examples are presented and discussed.

Acknowledgements.

This research was supported by the FCT project UID/MAT/00297/2013 (Centro de Matemática e Aplicações).

Numerical Approximation of Weakly Singular Integrals on a Triangle

Giada Serafini

University of Basilicata, v.le dell'Ateneo Lucano 10, 85100 Potenza, Italy
giada.serafini@unibas.it

Keywords. Numerical integration; Lagrange interpolation; Orthogonal polynomials.

In this talk it will be proposed an integration rule of "product"type for the numerical approximation of the following integrals

$$\int_{\mathbf{T}} K(x,y,s,t) f(x,y) \widetilde{\omega}(x,y) dxdy,$$

where the domain $\mathbf{T}$ is the triangle of vertices $(0,0),(0,1),(1,0)$, K is a weakly singular kernel of the type

$$K(x,y,s,t) = |s-x-y|^{\lambda} |t-x-y|^{\mu}, \quad -1 < \mu, \lambda \leq 0,$$

and $\widetilde{\omega}$ is a weight function of the form

$$\widetilde{\omega}(x,y) = (1-x-y)^b (x+y)^a x^{p-1} y^{q-1}, \quad p,q > 0,\ p+q+a > 0,\ b > -1.$$

This kind of integrals appears, for instance, in the numerical solution of bivariate integral equations (see [1], [2]). By means of a suitable transformation, we propose to approximate the integral by means of tensor product of univariate "product integration rules"based on Jacobi zeros [3]. The stability and convergence of the method are proved and some numerical tests, which confirm the theoretical estimates, are shown.

Acknowledgements. This research was supported by the *University of Basilicata* and by the *Centro Universitario Cattolico* (CUC).

References

[1] Mastroianni G., Milovanović G., Occorsio D. (2013), A Nyström method for two variables Fredholm integral equations on triangles, *Appl. Math. and Comput.*, Vol 219, pp. 7653–7662.

[2] Occorsio D., Russo M. G. (2011), Numerical methods for Fredholm integral equations on the square, *Appl. Math. and Comput.*, Vol 218, pp. 2318–2333.

[3] Smith W. E., Sloan I. H (1980), Product-integration rules based on the zeros of Jacobi polynomials, *SIAM J. Numer. Anal.* Vol 17 , pp. 1-13.

Special Session

"High Performance Computing in Modeling and Simulation"

Organizer:

William Spataro
University of Calabria, Italy

Parallel Processing of Genomics Data

Giuseppe Agapito, Pietro Hiram Guzzi and Mario Cannataro

University Magna Græcia of Catanzaro, Italy
agapito@unicz.it, hguzzi@unicz.it, cannataro@unicz.it

Keywords. genomics data; parallel computing; microarray; genotyping; statistical analysis.

The availability of high-throughput experimental platforms for the analysis of biological samples, such as mass spectrometry, microarrays and Next Generation Sequencing, have made possible to analyze a whole genome in a single experiment. Such platforms produce an enormous volume of data per single experiment, due to their capability to scan hundred thousands of markers at the time, thus the analysis of this enormous flow of data poses several challenges in term of data storage, preprocessing, and analysis. To face those issues, efficient, possibly parallel, bioinformatics software need to be used to preprocess and analyze data, for instance to highlight genetic variation associated with complex diseases.

In this paper we present a parallel algorithm for the parallel preprocessing and statistical analysis of genomics data, able to face high dimension of data and allowing efficient data analysis. The proposed system is able to find statistically significant biological markers showing good speed-up and scalability. The current algorithm extends the coreSNP system [1] and has been implemented as a massively parallel service.

Acknowledgements.
This work has been partially supported by the following research project funded by the Italian Ministry of University and Research (MIUR): PON03PE_00001_1 BA2Know-Business Analytics to Know.

References

[1] PH Guzzi, G Agapito, M Cannataro. coreSNP: Parallel processing of microarray data. IEEE Transactions on Computers, 63 (12), 2961-2974.

Energy-efficient workload management in distributed Data Centers leveraging autoregressive models

Albino Altomare, Eugenio Cesario, Carlo Mastroianni

ICAR-CNR, Rende (CS), Italy
altomare@icar.cnr.it, cesario@icar.cnr.it, mastroianni@icar.cnr.it

Keywords. Energy-aware Clouds; Regression Models; Green Computing.

The opportunity of using Cloud resources on a pay-as-you-go basis, the availability of powerful data centers and high bandwidth connections are speeding up the success and popularity of Cloud systems, which is making on-demand computing a common practice for many enterprises and scientific communities. The reasons for this success include natural business distribution, the need for high availability and disaster tolerance, the sheer size of their computational infrastructure, and/or the desire to provide uniform access times to the infrastructure from widely distributed client sites. Nevertheless, the expansion of large data centers is resulting in a huge rise of electrical power consumed by hardware facilities and cooling systems. Consequently, the efficient utilization of resources in the data centers is essential to reduce costs and energy consumption, while satisfying performance constraints and Service Level Agreement established with users. To deal with this issue, the geographical distribution of Data Centers is becoming a challenging issue to achieve energy efficiency and cost reduction in Cloud systems, whose adoption is rapidly increasing. In fact, it can expose many opportunities for optimizing energy consumption and costs by intelligently distributing the computational workload. This paper proposes an approach for energy-aware workload assignments and migrations, driven by regressive models. In particular, the energy consumption can be reduced by an optimized distribution of the workload among geographically distributed Data Centers, where migrations are scheduled taking into account workload predictions both within single sites and across the whole infrastructure. Preliminary experimental results show encouraging benefits in terms of energy saving.

Acknowledgements. This research was partially supported by the MIUR project DOMUS (PON03PE_00050_2).

References

[1] Mastroianni C., Meo M, Papuzzo G. (2013) Probabilistic Consolidation of Virtual Machines in Self-Organizing Cloud Data Centers. *IEEE Transactions on Cloud Computing*, Vol. 1(2), pp. 215–228.

[2] Altomare A., Cesario E. (2015) Predictive Models for Energy-Efficient Clouds: An Analysis on Real-Life and Synthetic Data. In Proceedings of the *14th IEEE International Conference on "Ubiquitous Computing and Communications", IUCC 2015* (ed. by IEEE), Liverpool (UK), pp. 1538–1543.

Characterization of one-dimensional cellular automata rules through topological network features

Lou D'Alotto, Clara Pizzuti

Department of Mathematics and Computer Science, York College, City University of New York, Jamaica, NY 11451, USA
National Research Council of Italy, Institute for High performance Computing and Networking, Via P. Bucci 7-11C, 87036 Rende (CS), Italy
ldalotto@bc.cuny.edu, pizzuti@icar.cnr.it

Keywords. one-dimensional cellular automata; Wolfram classification; Gilman classification.

Cellular automata are discrete computational systems having enormous potentials in modeling complex systems. Since their introduction by von Neuman they have attracted researchers from different fields and extensively studied. Wolfram, especially, investigated the dynamic behavior of one-dimensional automata and defined four types of behavior: homogeneous (Class I), periodic (Class II), chaotic (Class III) and complex (Class IV). This classification characterizes rules of each class by using parameters obtained by computer simulations. A different classification of linear automata into three classes $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$, has been proposed by Gilman. It is based on a measure theoretic classification approach that assigns a rule to a class by considering the probability of choosing a configuration that will stay close to a fixed initial configuration after the evolution of that rule for a time period. The relationship between Wolfram and Gilman classifications is not clear. Gilman asserts that Classes I and II lie in $\mathcal{A} \cup \mathcal{B}$, Class IV cannot be in $\mathcal{A}$ or $\mathcal{C}$, thus it must be in $\mathcal{B}$ and that Class III could be in $\mathcal{C}$. In this paper we investigate the relation between Wolfram and Gilman classes by exploiting the network representation of one-dimensional cellular automata. Each elementary rule is modeled with a network obtained by evolving the rule for a number of steps by starting from a random initial configuration. Some topological features of the graph generated after the evolution are computed and used to characterize the rules. Classification models by using machine learning classification methods are built and trained on the four Wolfram's classes already known. Then classification of Gilmans' rules in one of the four classes of Wolfram are obtained by applying the models to each rule.

References

[1] Wolfram W. (1994) *Cellular automata and complexity.* Addison-Wesley.
[2] Gilman R. H. (1987) Classes of Linear Automata. *Ergodic Theory and Dynamical Systems*, Vol. 7, pp. 105–118.

Scalable asynchronous execution of cellular automata

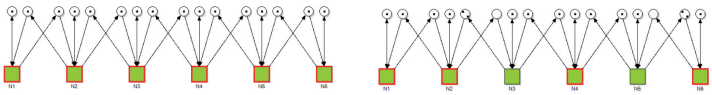
Gianluigi Folino, Andrea Giordano and Carlo Mastroianni

ICAR-CNR,
folino,giordano,mastroianni@icar.cnr.it

Keywords. space-aware applications; communication overhead; cellular automata; parallel computation.

The performance and scalability of cellular automata, when executed on parallel/distributed machines, are limited by the necessity of synchronizing all the nodes at each time step, i.e., a node can execute only after the execution of the previous step at all the other nodes. However, in many novel and increasingly popular applications of cellular automata, such as smart city applications, simulation of natural phenomena, etc., the synchronization requirements can be relaxed. In particular, a node can execute one step after synchronizing with a limited number of neighbor nodes. In this fashion, different nodes can execute different time steps. This can be a notable advantageous in scenarios in which the execution times can be different and variable, due to the heterogeneity of machines and/or data and/or executed functions. Indeed, a longer execution time at a node does not slow down the execution at all the other nodes but only at the neighbor nodes. This is particularly advantageous when the nodes that act as bottlenecks vary during the application execution. The goal of the paper is to analyze the benefits that can be achieved with the described asynchronous implementation of cellular automata, when compared to the classical all–to–all synchronization pattern. The performance and scalability have been evaluated through a Petri net model and for a real case scenario, i.e., the simulation of a landslide.

The Petri net model is also useful to better illustrate the execution strategy. In the case of a mono-dimensional cellular automaton, the parallel computation process, and the synchronization barrier among nodes, can be represented by the Petri net model depicted in Figure 1(a), in a sample scenario with six parallel nodes. Six Petri net transition, labeled as N1–N6, correspond to the parallel nodes, and the firing of a transition corresponds to the execution of the application on the corresponding node.



(a) (b)

Fig. 1. Petri net representing the execution of tasks at six parallel nodes. In (a) all the nodes are ready to execute. After execution at nodes N3, N4 and N5, the state of the Petri net is the one depicted in (b): N1, N2 N4 and N6 are ready to execute, N3 and N5 must wait for the execution at nodes N2 and N6, respectively.

Lava-flow hazard with optimized non-uniform grid of vents

Federica Lucà (1), Rocco Rongo (2, 3), Valeria Lupiano (4), Giulio Iovine (3)

1) CNR-ISAFOM, Rende, Italy
2) University of Calabria - Dept. of Mathematics and Computer Science, Rende, Italy
3) CNR-IRPI, Cosenza, Italy
4) University of Calabria - Dept. of Biology, Ecology, and Earth Sciences, Rende, Italy
federica.luca@isafom.cnr.it, rongo@unical.it, lupiano@unical.it, iovine@irpi.cnr.it

Keywords. Cellular Automata; Parallel computing; Spatial simulated annealing.

The aim of the study is to assess lava-flow hazard at Mt. Etna by the CA-model SCIARA [1, 2] in a parallel environment, introducing an optimization algorithm to integrate a uniform distribution of 1006 vents with 500 additional sources. Vents have iteratively been added at steps of 50 through spatial simulated annealing, using slope roughness as weigh function. For each vent, 41 types of simulation have been executed to take into proper account the potential behaviour of the volcano in terms of volume and duration, based on historical records.

Lava-flow hazard has been computed by adapting an approach recently employed for landslide hazard [3, 4], assigning each lava-flow simulation: i) a spatial likelihood of vent opening, depending on the proximity to structural weaknesses; ii) a magnitude probability, depending on the type of eruption; iii) a temporal probability of source activation for each temporal frame (up to 100 y), based on historical occurrences in the past 400 years. By overlapping the simulated lava flows and combining their probabilities, hazard maps have been obtained and the sensitivity with respect to the number of additional vents has been investigated.

References

[1] Crisci G.M., Iovine G., Di Gregorio S., Lupiano V. (2008) Lava-flow hazard on the SE flank of Mt. Etna (Southern Italy). *Journal of Volcanology and Geothermal Research,* Vol. 177, pp. 778–796.

[2] Rongo R., DAmbrosio D., Iovine G., Lucà F., Lupiano V., Bogolan V.P., Spataro W. (in press) A probabilistic approach to hazard mapping based on computer simulations. An example for lava flows at mount Etna. *Computer Modeling in Engineering & Sciences.*

[3] Lucà F., Avolio M.V., DAmbrosio D., Crisci G.M., Lupiano V., Robustelli G., Rongo R., Spataro W (2013) High detailed debris flows hazard maps by a cellular automata approach. In *Landslide Science and Practice,* Vol. 6 (ed. by Margottini C., Canuti P., Sassa K.), Berlin (German), pp. 733–737.

[4] Lucà F., D'Ambrosio D., Robustelli G., Rongo R., Spataro W. (2014) Integrating geomorphology, statistic and numerical simulations for landslide invasion hazard scenarios mapping: An example in the Sorrento Peninsula (Italy). *Computers & Geosciences*, Vol. 67, pp. 163–172.

A Cellular Automata Based FPGA Realization of a New Metaheuristic Bat-Inspired Algorithm

Pavlos Progias[1], Angelos A. Amanatiadis[1], William Spataro[2], Giuseppe A. Trunfio[3], and Georgios Ch. Sirakoulis[1]

[1] Department of Electrical and Computer Engineering, Democritus University of Thrace, Xanthi 67100, Greece
pavlprog@ee.duth.gr, aamanat@ee.duth.gr, gsirak@ee.duth.gr
[2] Department of Mathematics and Computer Science, University of Calabria, Rende (CS), 87036, Italy
spataro@unical.it
[3] Department of Architecture, Planning and Design, University of Sassari, Alghero (SS), 07041 Italy
trunfio@uniss.it

Keywords. Bat Algorithm; Cellular Automata; Field Programmable Gate Array (FPGA); Metaheuristic Optimization; Bio-inspired Computing.

Optimization algorithms are often inspired by processes occuring in nature, such as animal behavioral patterns. The main concern with implementing such algorithms in software is the large amounts of processing power they require. For example, modelling the behavior of a large group of wild animals in discrete time steps, would mean a huge amount of calculations for each time step, even if each unit of the pack only makes simple calculations. In contrast to software code, that can only perform calculations in a serial manner, an implementation in hardware, exploiting the inherent parallelism of single-purpose processors, can prove to be much more efficient both in speed and energy consumption. Furthermore, the use of Cellular Automata (CA) in such an implementation would be efficient both as a model for natural processes, as well as a computational paradigm implemented well on hardware. In this paper, we propose a VHDL implementation of a metaheuristic algorithm inspired by the echolocation behavior of bats. More specifically, the CA model is inspired by the metaheuristic algorithm proposed earlier in the literature, which be could considered at least as efficient than other existing optimization algorithms. In this work, we propose a CA implementation based on the aforementioned algorithm on a Stratix II FPGA. The goal of the paper is to design and implement a hardware-based model, designed to execute in a parallel way in order to produce valuable information in a short period of time, that will have less stringent requirements on computational resources for execution than its software-based countepart. In addition, we created software code that can produce the VHDL implementation of our model on a CA of arbitrary dimensions, making our work easily scalable. The function of our FPGA is explained in full detail and results of our simulations are also demonstrated proving in a quantitative way how proposed hardware meets the algorithm' constraints.

Wind speed interpolation for hydrological modeling in complex topography area

Giovanni Ravazzani, Silvio Davolio, Alessandro Ceppi, Alessandro Fiore

Politecnico di Milano, Dipartimento di Ingegneria Civile e Ambientale, Milano, Italy
Consiglio Nazionale delle Ricerche, Istituto di Scienze dell'Atmosfera e del Clima, Bologna, Italy
Politecnico di Milano, Dipartimento di Ingegneria Civile e Ambientale, Milano, Italy
Politecnico di Milano, Dipartimento di Ingegneria Civile e Ambientale, Milano, Italy
giovanni.ravazzani@polimi.it, s.davolio@isac.cnr.it,
alessandro.ceppi@polimi.it, alessandro.fiore@mail.polimi.it

Keywords. Wind speed interpolation; Complex topography; Hydrological modelling.

Wind speed and direction are fundamental data in many fields such as power generation, and hydrological modeling. Within the hydrological domain, among other uses, wind data are used to compute evapotranspiration and correct precipitation measurement. Wind measurements are sparse, hence spatial interpolation of wind data is required. In mountainous area with complex topography, accurate interpolation of wind data should consider topographic effects. The wind field can be generated by several methods, including: 1) applying a physically based, full atmospheric model which satisfy all relevant momentum and continuity equations, 2) applying an atmospheric model in which1only mass continuity is satisfied, 3) interpolation using wind-speed and direction observations in conjunction with empirical wind-topography relationships. Due to computational constraints, methods 1 and 2 can not be applied for long time simulations like the ones required for assessing climate change impacts. The aim of this work is to compare different techniques to interpolate wind speed in a complex topography area. The subject area is the upper Po River basin and covers 38 000 km^2. This is predominantly an alpine region located in Northern Italy that is bounded on three sides by mountain chains covering 73% of its territory. Impact of wind data interpolation accuracy is assessed by running the FEST-WB model (flash Flood Event based Spatially distributed rainfall runoff Transformation, including Water Balance), a spatially distributed model that computes the main processes of the hydrological cycle: evapotranspiration, infiltration, surface runoff, flow routing, subsurface flow, and snow melt and accumulation. Results show that the use of empirical methods based on wind-topography relationships provide good accuracy for river basin hydrological analysis at a fraction of the computational cost required by physically based atmospheric models.

Algorithms for the analysis and characterization of convective structures relative to extreme rainfall events.

Pietro Sabatino, Francesco Chiaravalloti, Giuseppe Fedele, Salvatore Gabriele

CNR - ICAR, Via P. Bucci 41/C, 87036 Rende (CS), Italy
CNR - IRPI, Via Cavour, 4-6, 87036 Rende (CS), Italy
UNICAL - DEIS, Via Pietro Bucci 42/C, 87036 Rende (CS), Italy
CNR - IRPI, Via Cavour, 4-6, 87036 Rende (CS), Italy
pietro.sabatino@icar.cnr.it, f_chiaravalloti@yahoo.it,
giuseppe.fedele@unical.it, salvatore.gabriele@irpi.cnr.it

Keywords. Numerical weather prediction; Machine Learning; Image processing.

Among many weather phenomena, convective storms are one of the most dangerous since they are able to cause, in a relatively small time window, great damages. Convective precipitations are in fact characterized by relatively small spatial and temporal scales, and as a consequence, the task of forecasting such phenomena turns out to be an elusive one. Nonetheless, given their dangerousness, the identification and tracking of meteorological convective systems is of paramount importance, and it is the subject of several research studies, that in particular emphasizes the early detection of the areas where deep convection is about to appear. Indeed, in order for deep convection to occur, there must be adequate atmospheric conditions in terms of moisture and thermal lapse rate. At least in principle, these conditions can be extrapolated in real time, or nearly real time, from the data coming from modern geostationary meteorological satellites, such as METEOSAT, that are able to characterize atmospheric conditions in terms of radiance, and many works in literature exploit this possibility by using technique of image processing applied to data coming from geostationary satellites, Walker et al. [1]. The aim of the present work, is to perform a systematic comparison of various techniques apt to the task of monitoring and characterizing of convective clouds, they analyze meteorological satellite images and data in order to evaluate the potential occurring of strong precipitation. Techniques considered include numerical, machine learning, image processing and ensemble based, Williams et al. [2] . The techniques are tested on data coming from real convective events captured in the last years on the Italian peninsula by the METEOSAT meteorological satellites.

Acknowledgements. This research was supported by the CNR project RAMSES (RAilway Meteorological SEcurity System) co-funded by RFI S.p.A.

References

[1] John R. Walker, Wayne M. MacKenzie Jr., John R. Mecikalski, and Christopher P. Jewett (2012) An Enhanced Geostationary SatelliteBased Convective Initiation Algorithm for 02-h Nowcasting with Object Tracking. *J. Appl. Meteor. Climatol.*, 51, 19311949.

[2] Williams, J. K., Ahijevych, D. A., Kessinger, C. J., Saxen, T. R., Steiner, M., & Dettling, S. (2008, January). A machine learning approach to finding weather regimes and skillful predictor combinations for short-term storm forecasting. In *AMS 6th Conference on Artificial Intelligence Applications to Environmental Science and 13th Conference on Aviation, Range and Aerospace Meteorology.*

Accelerating a Three-dimensional Eco-Hydrological Cellular Automaton on GPGPU with OpenCL

Alfonso Senatore[1] , Donato DAmbrosio[2] , Alessio De Rango[2] , Rocco Rongo[2] , William Spataro[2], Salvatore Straface[1], Giuseppe Mendicino[1]
{alfonso.senatore, d.dambrosio, spataro}@unical.it

[1] Department of Environmental and Chemical Engineering, University of Calabria, Rende (CS), Italy
[2] Department of Mathematics and Computer Science, University of Calabria, Rende (CS), Italy

Keywords. Modelling; Cellular Automata; GPGPU

This work presents an effective implementation of a well-known numerical model for complete eco-hydrological model (EHCA) based on the approach of eXtended Cellular Automata on Graphical Processing Units (GPU) based on the OpenCL (Open Computing Language) for standard computation to the GPUs but also on heterogeneous platforms (joint CPUs and GPUs). In particular, the framework models the interactions between water and ecosystems, it includes the transpiration and plant water usage, the influence that the vegetation has on the streamflow, the feedbacks between ecological processes and the hydrological cycle, the solar irradiance, the vegetation dynamics, the CO2, and the energy fluxes. Different types of parallel implementations were carried out (e.g., use of fast local memory, loop unrolling, etc), showing increasing significant performance improvements in terms of speedup, adopting also some original optimizations strategies. Moreover, numerical analysis of results (i.e., comparison of CPU and GPU outcomes in terms of rounding errors) have proven to be satisfactory. Experiments were carried out with a hardware equipment consisting of a workstation with two CPUs (Intel Xeon E5440 at 2.83GHz), one GPU AMD R9 280X and one GPU nVIDIA Tesla k20c. The results obtained on the EHCA model have been extremely positive, but further testing should be performed to assess the functionality of the adopted strategies on other complete models and their ability to fruitfully exploit parallel systems resources.

References

[1] Mendicino G, Senatore A, Spezzano G (2006) Three dimensional unsaturated flow modeling using cellular automata. *Water Resources Research*, Vol. 42(11).
[2] Spataro D, DAmbrosio D, Filippone G, Rongo R, Spataro W, Marocco D (2013) Efficient application of GPGPU for lava flow hazard mapping, *Journal of Supercomputing*, Vol. 65 (2), pp. 630-644.

Special Session
"Intractable Problems and Approximation Algorithms"

Organizers:

Adil Erzin
Yuri Kochetov
Sobolev Institute of Mathematics
Novosibirsk State University, Russia

Approximation Algorithms for the Min-Power Symmetric Connectivity Problem

Adil Erzin, Nenad Mladenovic, Roman Plotnikov

Sobolev Institute of Mathematics, Novosibirsk, Russia
University of Valenciennes and Hainaut-Cambresis, Famars, France
Sobolev Institute of Mathematics, Novosibirsk, Russia
adilerzin@math.nsc.ru, nenadmladenovic12@gmail.com, nomad87@ngs.ru

Keywords. Wireless networks; NP-hard problem; variable neighborhood search.

We investigate the problem, which occurs in many wireless networks while minimizing the communication power consumption. It can be formulated as follows. A simple undirected edge-weighted graph is given. For any spanning subgraph of this graph suppose that the weight of a vertex is the maximum weight of its incident subgraph's edges. The problem is to find such spanning subgraph of a given graph that the sum of vertex weights is minimum.

This problem is known as *Min-Power Symmetric Connectivity Problem* (MPSCP) [1]. The problem MPSCP is strongly NP-hard [1, 3], therefore construction and analysis of efficient approximation algorithms is one of the most important issues regarding this problem.

In this paper we propose new heuristics based on the variable neighborhood search metaheuristic [2] for the approximation solution of MPSCP. We have performed a simulation where all proposed algorithms have been executed on randomly generated test samples. New algorithms have been compared with the approaches proposed earlier [3, 4]. The results, which demonstrate a high efficiency of the proposed algorithms, will be presented in the full version of the paper.

References

[1] Althaus, E. et al. (2006) *Power efficient range assignment for symmetric connectivity in static ad hoc wireless networks*, Wireless Networks 12 (3) pp. 287–299.

[2] Hansen, P., Mladenovic, N. (2001) *Variable neighborhood search: Principles and applications*, European Journal of Operational Research 130 pp. 449–467.

[3] Erzin, A., Plotnikov, R., Shamardin, Y. (2013) *On some polynomially solvable cases and approximate algorithms in the optimal communication tree construction problem*, Journal of Applied and Industrial Mathematics 7 pp. 142–152.

[4] Erzin, A., Plotnikov, R. (2015) *Using VNS for the optimal synthesis of the communication tree in wireless sensor networks*, Electronic Notes in Discrete Mathematics 47 pp. 21–28.

Comparative Analysis of Regular Covers with One or Two Types of Sectors

Adil Erzin, Lydia Osotova

Sobolev Institute of Mathematics, Novosibirsk, Russia
Novosibirsk State University, Novosibirsk, Russia
adilerzin@math.nsc.ru, lidochkaprivet@gmail.com

Keywords. Regular covers; density; sectors.

The *cover* of a plane domain is such set of figures that each point of the domain belongs to at least one figure in the cover. The coverage *density* is the ratio of the sum of the areas of the figures in the cover to the area of the covered domain. In many applications it is required to find a min-dense cover.

In the *regular* covers, the plane region is split into the equal polygons (*tiles*), and all the tiles are covered uniformly. Therefore, in order to estimate the density of the regular cover it is sufficient to consider the covering of one tile. The density of the regular cover depends on the shape of the tile, the types of the figures, and the number of the figures that cover one tile.

In [1] introduced a classification of the regular covers. Evidently, it is correct to compare the covers in the same class. In [2] a regular covering of the plane having the minimum density, which uses equal disks, is suggested. In [3] proposed a regular cover with the disks of two radii, the density of which tends to 1.0189 when the number of disks tends to infinity. It also uses the cover which introduced in [2] as a fragment. The cover proposed in [3] inspired us to search for the similar cover with the sectors of two types. We have found the density function, depending on the number of sectors involved in the coverage of one tile. When the number of sectors involved in the coverage of one tile is at most 27 the density of the proposed cover is less than 1.0189.

Then we compare five different covers with sectors of one or two types and get the best coverage model for each number of sectors involved in the coverage of one tile. In particular, the density of two considered covers tends to 1 when the number of sectors covering one tile tends to infinity.

References

[1] Zalyubovskiy V., Erzin A., Astrakov S., Choo H. (2009) Energy-efficient area coverage by sensors with adjustable ranges. *Sensors*, Vol. 9, No. 4, pp. 2446–2460.

[2] Kershner R. (1939) The number of circles covering a set. *American Journal of Mathematics*, Vol. 61, No. 3, pp. 665–671.

[3] Fejes Tóth G. (1995) Covering the Plane with Two Kinds of Circles. *Discrete & Computational Geometry*, Vol. 13, No. 3, pp. 445–457.

The TSP-approach to approximate solving the m-Cycles Cover problem

Edward Kh. Gimagi, Ivan Rykov, Oxana Tsidulko

Sobolev Institute of Mathematics, Novosibirsk, Russia
Novosibirsk State University, Novosibirsk, Russia
gimadi@math.nsc.ru, rykovweb@gmail.com, tsidulko.ox@gmail.com

Keywords. m-Cycles Cover problem; TSP; approximation algorithm.

We study the m-Cycles Cover (m-CCP) problem which is a natural generalization of the well-known traveling salesman problem (TSP). Given a complete weighted graph G, the problem is to find m cycles of extreme total weight, such that every vertex in G belongs to exactly one cycle. Note that the 1-CCP is the TSP. The m-CCP is strongly NP-hard. The MIN m-CCP remains NP-hard even in Metric or Euclidean statements [1]. Therefore our goal is to construct approximation algorithms with proven performance guarantees for the problem.

We suggest the TSP-approach to generate approximate solutions for the m-CCP [2]. First we construct an approximate solution for the TSP. Then we solve the auxiliary problem to find the best partition of the Hamiltonian cycle into a set of m disjoint chains which further are completed to m desired cycles.

Here we present a number of successful transformations of known TSP approximations into m-CCP approximation algorithms. Using the TSP-approach we've obtained asymptotically optimal algorithms for the Euclidean MAX m-CCP and for m-CCP on the Euclidean integer lattice and restricted graph's diameter. We've got algorithm for symmetric MAX m-CCP out of the well known 3/4-approximation for TSP, and algorithms for t he metric MAX m-CCP, using 5/6 and 7/9 TSP approximations. The algorithms for MIN TSP seem to be less promising for our approach. Still we've constructed an asymptotically optimal algorithm solving the MIN m-CCP on random inputs uniformly distributed in $[0, 1]$.

Acknowledgements.

This research was supported by Russian Foundation for Basic Research grants no. 16-31-00389 and 15-01-00976.

References

[1] M. Yu. Khachai, E. D. Neznakhina (2015) *A polynomial-time approximation scheme for the Euclidean problem on a cycle cover of a graph.* Proceedings of the Steklov Institute of Mathematics 289(1), pp 111–125

[2] E. Kh. Gimadi, I. A. Rykov (2015) *Asymptotically optimal approach to the approximate solution of several problems of covering a graph by nonadjacent cycles.* Trudy Inst. Mat. i Mekh. UrO RAN 21(3), pp 89–99

Approximability of the d-dimensional Euclidean Capacitated Vehicle Routing Problem

Michael Khachay, Roman Dubinin

Krasovskii Institute of Mathematics and Mechanics
Ural Federal University, Ekaterinburg Russia
Omsk State Technical University
Omsk, Russia mkhachay@imm.uran.ru, machas_briefen@mail.ru

Keywords. Euclidean Capacitated Vehicle Routing Problem; Polynomial Time Approximation Scheme.

The Capacitated Vehicle Routing Problem is the well known special case of Vehicle Routing Problem [1], which is widely adopted in operations research. In its simplest setting, the VRP can be treated as the combinatorial optimization problem aiming to design the cheapest collection of delivery *routes* of a vehicle of a given *capacity* q from single or multiple dedicated points (*depots*) to a set of customers (*clients*) given by their spacial locations.

The CVRP is strongly NP-hard and APX-complete being close to several well known NP-hard combinatorial problems. For instance, Traveling Salesman Problem (TSP) is a subclass of the CVRP such that a depot is collocated with one of clients and $q \geq n$. Almost all known special cases of the CVRP (except the case when $q \leq 2$) are also NP-hard even in Euclidean spaces of finite dimension.

Most approximation results for CVRP are obtained for the Euclidean plane. One of the first studies of two-dimensional Euclidean CVRP has been due to Haimovich and Rinnooy Kan [2], who presented several heuristics for this problem leading to the first PTAS for $q = O(\log \log n)$.

In this paper, we extend the results obtained in [2, 3] to the case of any fixed dimension $d > 1$ and fixed number m of depots. Actually, we propose a new Efficient Polynomial Time Approximation Scheme (EPTAS) for the Euclidean CVRP, for which capacity q, the number of depots m, and dimension $d > 1$ are fixed. The algorithm proposed remains PTAS for the problem with fixed m, $d > 1$, and $q = O(\log \log n)^{1/d}$.

Acknowledgements. This research was supported by the Russian Science Foundation, grant no. 14-11-00109.

References

[1] Toth P. and Vigo D (2001) *The Vehicle Routing Problem*. Society for Industrial and Applied Mathematics, Philadelphia.

[2] Haimovich M. and Rinnooy Kan A. H. G. (1985) Bounds and Heuristics for Capacitated Routing Problems *Mathematics of Operations Research*, Vol. 10, pp. 527–542.

[3] Khachay M. and Zaytseva H. (2015) Polynomial Time Approximation Scheme for Single-Depot Euclidean Capacitated Vehicle Routing Problem *LNCS*, Vol. 9486, pp. 178–190.

Towards a PTAS for the Generalized TSP in Grid Clusters

Michael Khachay, Katherine Neznakhina

Krasovsky Institute of Mathematics and Mechanics
Ural Federal University, Ekaterinburg Russia
mkhachay@imm.uran.ru, eneznakhina@yandex.ru

Keywords. Generalized Traveling Salesman Problem; Polynomial time approximation scheme.

The Generalized Traveling Salesman Problem (GTSP) [1] is a combinatorial optimization problem, which is to find a minimum cost cycle visiting at least one node (city) in each given cluster. We consider a geometric case of this problem, where n nodes are given inside the integer grid (in the Euclidean plane), each grid cell has size 1×1. Clusters are induced by 'populated' cells. Even in this special setting, the GTSP remains intractable enclosing the classic Euclidean TSP on the plane. Recently [2], it was shown that the problem has $(1.5 + 8\sqrt{2} + \varepsilon)$-approximation algorithm with complexity bound depending polynomially on n and k, where k is the number of clusters.

We propose two approximation schemes for this problem. In the first scheme, we round the instance by dividing the populated cells by subsquares and moving any initial node to the nearest center. Then, for every set of k nodes chosen in a special way, we find an exact TSP solution using dynamic programming. In the second one, we find $(1 + 1/c)$-approximate traveling salesman tour in $O(k^3(\log k)^{O(c)})$ for every hitting set for the given clusters using the famous algorithm obtained by S.Arora. The first scheme is a PTAS for $k = O(\log n$ while the second one is a PTAS for $k = n - O(\log n)$.

Acknowledgements.

This research was supported by Russian Science Foundation, grant no. 14-11-00109.

References

[1] Laporte, G., Asef-Vaziri, A., Sriskandarajah, C. (1996) Some applications of the gener- alized traveling salesman problem. *Journal of Operational Research Society*, Vol. 47, pp. 1461–1467.

[2] Bhattacharya B., Cústić A., Rafiey Ak., Rafiey Ar., and Sokol V. (2015) Approximation Algorithms for Generalized MST and TSP in Grid Clusters. *LNCS*, Vol. 9486, pp. 110–125.

Optimization with quadratic support functions in nonconvex smooth optimization

Oleg Khamisov

Melentiev Institute of Energy Systems, 664033 Irkutsk, Lermontov street 130, Russia
khamisov@isem.irk.tu

Keywords. Global optimization, Lipschitz derivatives, quadratic support functions, branch and bound method.

The main subject of the talk is global minimization of twice continuously differentiable function with Lipschitz second derivatives over a polytope. We suggest a branch and bound method with polytopes as partition elements. Due to the Lipschitz property of the objective function we can construct a quadratic support minorant at each point of the feasible set. Global minimum of of this minorant provides a lower bound of the objective over given partition subset. The main advantage of the suggested method consists in the following. First quadratic minorants usually are nonconvex and we have to solve auxiliary global optimization problem. This problem is reduced to a mixed 0-1 linear programming problem and can be solved by an advanced 0-1 solver. Then we show that the quadratic minorants are getting convex as soon as partition elements are getting smaller in diameter. Hence, at the final steps of the branch and bound method we solve convex auxiliary quadratic problems. Therefore, the method accelerates when we are close to the global minimum of the initial problem.

This technique is extended to some smooth nonconvex optimization problems. We also discuss several ways of calculating the Lipschitz constant.

Convergence conditions are given and results of numerical experiments are presented.

Acknowledgements.

This research was supported by RFBR grant 15-07-08986

References

[1] Khamisov O. (1999) On optimization properties of functions with a concave minorant. *J. Globl. Optim.*, Vol. 14, pp. 795–101.

[2] Khamisov O. (2013) Nonconvex optimization with nonlinear support functions. *Trudy IMM UrO RAN*, Vol. 19, No. 2,pp. 295–306. (in Russian)

Complexity and approximability for problem of stabbing of proximity graphs with minimum number of equal disks

Konstantin Kobylkin

Institute of Mathematics and Mechanics, Ural Branch of Russian Academy of Sciences, Sophya Kovalevskaya str. 16, Ekaterinburg, Russia
kobylkinks@gmail.com

Keywords. computational complexity; proximity graphs; approximability.

Computational complexity and approximability are studied for the problem of stabbing a structured set of straight line segments with the smallest cardinality set of disks of fixed radii $r > 0$ where the set of segments forms straight line embedding of possibly non-planar graph. This problem arises in physical network security analysis for telecommunication, wireless and road networks represented by geometric graphs based on euclidean distances between their vertices (proximity graphs). It can be formulated in the form of known Hitting Set problem over a structured set of euclidean r-neighbourhoods of segments (i.e. proximity graph edges). Being of interest computational complexity and approximability of Hitting Set over so structured sets of geometric objects did not get much focus in the literature. Strong NP-hardness is reported of the problem over classes of Delaunay triangulations, some of their connected subgraphs, half-θ_6 graphs and non-planar unit disk graphs as well as APX-hardness is given for non-planar graphs at different scales of r with respect to the longest graph edge length. Simple constant factor approximation algorithm is presented for the case where r is at the same scale as the longest edge length.

Acknowledgements.
The research is supported by Russian Science Foundation proj. 14-11-00109.

Local Search Heuristic for the Discrete Leader-Follower Problem with Multiple Follower Objectives

Yury Kochetov, Ekaterina Alekseeva, Mohand Mezmaz

Sobolev Institute of Mathematics, Novosibirsk, Russia
Novosibirsk State University, Novosibirsk, Russia
MARO, University of Mons, Belgium
jkochet@math.nsc.ru, katerina.alekseeva@gmail.com,
Mohand.MEZMAZ@umons.ac.be

Keywords. Bi-level programming; Stackelberg game; Local search.

In the bi-level optimization we deal with a two level hierarchical structure of decision making: upper level and lower level. These levels correspond to two decision makers called a leader and a follower. The leader plays at the upper level and the follower plays at the lower one. An upper level decision is influenced by a decision of the lower level. The bi-level programs can be considered as Stackelberg games or mathematical programs with optimization problems in the constraints.

In this paper we tackle a discrete leader-follower problem with multiple follower objectives. In such a case we deal with a set of Pareto efficient solutions of the follower rather than a single optimal one. To calculate leader objective function value, we need to select the best solution out of a potentially large set of efficient follower solutions. To avoid the enumeration of the whole set of Pareto solutions, we formulate an auxiliary mixed integer problem to optimize the leader objective function over the Pareto set. We propose a new exact method to solve the problem where local search heuristics are used to generate cuts and to improve lower and upper bounds of the optimum to the auxiliary problem.

In the case of the bi-level problem with multiple follower objectives, we face with ill-posed problem. Moreover, we assume that the follower variables can be included into the upper level constraints. Thus, we define feasible and optimal solutions to the problem for optimistic and pessimistic cases and design local search heuristics for finding near optimal solutions. The efficiency of the proposed approach is evaluated on a discrete $(r \mid p)$-centroid problem with two objectives of the follower.

Acknowledgement

This research was supported by the RSF grant 15-11-10009.

The Lower Bound on Complexity of Parallel Branch-And-Bound Algorithm for Subset Sum Problem

Roman Kolpakov[1,2], Mikhail Posypkin[2]

Lomonosov Moscow State University, GSP-1, Leninskie Gory, Moscow, Russia
Dorodnicyn Computing Centre, FRC CSC RAS, Vavilov st. 40, Moscow, Russia
foroman@mail.ru, mposypkin@gmail.com

Keywords. Complexity; Knapsack Problem; Parallel Branch-and-Bound.

The subset sum problem is a particular case of the Boolean knapsack problem where each item has the price equal to its weight:

$$f(x) = \sum_{i=1}^{n} w_i x_i \to \max, \sum_{i=1}^{n} w_i x_i \le C, x_i \in \{0,1\}, i = 1, \ldots, n.$$

Informally this problem can be stated as searching for most dense packing of a set of items into a box with limited capacity. Despite simple formulation this problem appears to be NP-hard and its resolution by the Branch-and-Bound (B&B) method requires large amount of computational resources. Parallel and distributed computing can help to significantly reduce the running time. Recently coarse-grain parallelization approaches to B&B method attracted some attention due to the growing popularity of weakly-connected distributed computing platforms. In this paper we consider one of such approaches. One of the processors (manager) performs some number of B&B steps on the first stage. On the second stage, the obtained subproblems are sent to other processors, one subproblem per processor. Then processors solve the received subproblems completely, the manager collects all the obtained solutions and chooses the optimal one.

We formally define the parallel execution model for this algorithm and the notion of complexity. The model assumes the unlimited number of processors. We study the parallel complexity for a series of subset sum problems with variable capacity $C = ka$. We show that the asymptotic behaviour of the minimal parallel complexity remains $2^{n/2}/\sqrt[4]{n}$ for a wide range of capacities $n/4 \le k \le 3n/4$. For marginal values of k, $1 \le k \le \frac{3-\sqrt{5}}{4}n$, $\frac{1+\sqrt{5}}{4}n \le k \le n$ the situation changes: the minimal parallel complexity asymptotically equals to $\binom{\lfloor n/2 \rfloor}{k+1}$.

Acknowledgements.

This research was supported by Russian Fund for Basic Research, grants 16-07-00458 and 15-07-03102.

The Upper Bound on the Complexity of Branch-and-Bound with Cardinality Bound for Subset sum Problem

Roman Kolpakov[1,2], Mikhail Posypkin[2,3], Si Thu Thant Sin[3]

[1]Lomonosov Moscow State University, GSP-1, Leninskie Gory, Moscow, Russia
[2]Dorodnicyn Computing Centre, FRC CSC RAS, Vavilov st. 40, Moscow, Russia
[3]National Research University of Electronic Technology - MIET
foroman@mail.ru, mposypkin@gmail.com, sithuthantsin86@gmail.com

Keywords. Complexity; Subset sum Problem; Branch-and-Bound Method.

One of the basic packing problems is a subset sum problem that consists in finding the most dense packing of items with weights $w_1, \ldots, w_n$ to a container with the given capacity C:

$$f(x) = \sum_{i=1}^{n} w_i x_i \to \max, \sum_{i=1}^{n} w_i x_i \le C, x_i \in \{0,1\}, i = 1, \ldots, n. \qquad (1)$$

Following common approach we assume item weights be positive integral values.

It was previously shown that the worst case complexity of a standard Branch-and-Bound for the problem (1) is never greater than

$$L_1(n) = 2\binom{n+1}{\lfloor n/2 \rfloor + 1} - 1. \qquad (2)$$

We consider an advanced B&B with an additional pruning rule: the sub-problem is discarded if the number of heaviest items that can be put to the container equals to the number of the most lightweight items that can be paced there. Such property ensures a unique choice for a selection of items and the sub-problem satisfying it can be resolved in one step. We show that the worst case complexity for the advanced B&B with the new pruning rule is

$$L_2(n) = 2\binom{n}{\lfloor n/2 \rfloor + 1} - 1. \qquad (3)$$

Bound (3) is asymptotically twice better than bound (2).

Acknowledgements.

This research was supported by Russian Fund for Basic Research, grants 16-07-00458 and 15-07-03102.

Optimal Recombination in Genetic Algorithms for Flowshop Scheduling Problems

Julia Kovalenko

Sobolev Institute of Mathematics, 4 Acad. Koptyug Ave., 630090 Novosibirsk, Russia
julia.kovalenko.ya@yandex.ru

Keywords. Flowshop problem; permutation; genetic algorithm; optimal recombination.

The classical flowshop scheduling problem with n jobs and m machines is defined as follows. Each of n jobs is to be sequentially processed on m machines. The processing times of jobs on machines are given. At any time, each machine can process at most one job and each job can be processed on at most one machine. In the permutation flowshop problem the order in which jobs are to be processed is the same for each machine. In the no-wait variation on the problem each job, once started, has to be processed without interruption until it is completed.

Flowshop scheduling problems are NP-hard combinatorial optimization problems. Exact techniques are only applicable to small-sized problems in practice. Therefore metaheuristics, in particular, genetic algorithms, are appropriate for these problems. Performance of genetic algorithms depends significantly upon the choice of the crossover operator, where the components of parent solutions are combined to build the offspring. Optimal Recombination Problem (ORP) consists in finding the best possible offspring as a result of a crossover operator, given two feasible parent solutions. Note that optimal recombination may be considered as a local search step in the space of populations of a genetic algorithm.

This work is devoted to complexity and solution method of the ORP for various variants of the flowshop scheduling problem with makespan criterion and criterion of maximum lateness. NP-hardness of this optimal recombination problem is proven. We build an algorithm for solving the ORP, using enumeration of all possible combinations of the maximal matchings in cycles of a special bipartite graph. It is shown that the ORP for the permutation flowshop scheduling problem is solvable in polynomial time for almost all pairs of parent solutions as the number of jobs n tends to infinity.

Acknowledgements.
This research is supported by the Russian Science Foundation grant 15-11-10009.

A Local search for a GRAPH CLUSTERING problem

Anna Navrotskaya, Victor Il'ev

Sobolev Institute of Mathematics, 4 Acad. Koptyug Ave., 630090 Novosibirsk, Russia
Omsk State University, 55-a Mira Ave., 644077 Omsk, Russia
nawrocki@ya.ru, iljev@mail.ru

Keywords. Graph clustering; local search; approximation algorithm.

The objective of the clustering problems is to partition a given set of objects into a family of subsets (named *clusters*) such that objects within a cluster are more similar to one another than objects in different clusters. The clustering is usually based on some similarity measure defined for the objects that may be different in the different problems.

One of most visual formalizations of clustering is GRAPH CLUSTERING, that is, grouping the vertices of a graph into clusters taking into consideration the edge structure of the graph whose vertices are objects and edges represent similarities between the objects. In GRAPH k-CLUSTERING the number of clusters does not exceed k and the goal is to minimize the number of edges between clusters and the number of missing edges within clusters. This problem is NP-hard for any fixed $k \geq 2$.

For approximate solving GRAPH k-CLUSTERING a local-search approach is used. In 2008 [1], applying a local-search strategy Coleman, Saunderson and Wirth proposed 2-approximation algorithm for GRAPH 2-CLUSTERING. Extending this strategy we propose a polynomial time approximation algorithm for GRAPH k-CLUSTERING with linear on k performance guarantee.

Acknowledgements.

This research was supported by the Russian Science Foundation grant 15-11-10009.

References

[1] Coleman T., Saunderson J., Wirth A. (2008) A local-search 2-approximation for 2 correlation-clustering. *Algorithms - ESA 2008: Lecture Notes in Computer Science*, Vol. 5193, pp. 308–319.

On a numerical solving of random generated hexamatrix games

Andrei Orlov, Alexander Strekalovskiy

Matrosov Institute for System Dynamics and Control Theory of SB RAS,
Lermontov str., 134, Irkutsk, Russia
anor@icc.ru, strekal@icc.ru

Keywords. Hexamatrix games; Global Search Theory; numerical solution.

As well known, the building of efficient methods and numerical finding equilibrium points in Game Theory problems is the current issue for the contemporary mathematical optimization theory and methods [1]. The situation is easy only for the simplest Matrix Games which can be reduced to two dual linear programming problems [2]. The first extension of a matrix game is a non-antagonistic two-player bimatrix game. Such a game already reduced to non-convex bilinear programming problem [2].

An even more difficult situation arises during the transition from two to three players. In that case we have a hexamatrix game (polymatrix game of three players) [3]. According to [3] the finding of Nash equilibrium in hexamatrix game is equivalent to non-convex mathematical optimization problem with a triple bilinear structure in the goal function and joint constraints.

In this work we propose to solve the latter problem with the help of Global Search Theory [4]. The Global Search consists of two principal stages: 1) a local search, which takes into account the structure of the problem under scrutiny; 2) the procedures based on Global Optimality Conditions, which allow to improve the point provided by the local search method.

The efficiency of methods developed for hexamatrix games is demonstrated by the results of computational solving of random generated test problems.

Acknowledgements.

This research was supported by the Russian Science Foundation (project No. 15-11-20015).

References

[1] Pang J.-S. (2010) Three modeling paradigms in mathematical programming. *Math. program. Ser.B.*, Vol. 125(2), pp. 297–323.

[2] Orlov A.V., Strekalovsky A.S. (2005) Numerical search for equilibria in bimatrix games. *Comput. Math. Math. Phys.*, Vol. 45(6), pp. 947–960.

[3] Strekalovsky A.S., Enkhbat R. (2014) Polymatrix games and optimization problems. *Autom. Remote Control*, Vol. 75(4), pp. 632–645.

[4] Strekalovsky A.S. (2003) *Elements of Nonconvex Optimization*. Nauka, Novosibirsk (in Russian).

On Three-Level Problem Of Competitive Pricing

Alexander Plyasunov, Artem Panin

Sobolev Institute of Mathematics, Pr. Akademika Koptyuga,4, 630090, Novosibirsk, Russia
apljas67@gmail.com, arteam1897@gmail.com

Keywords. Three-level problem; competitive pricing; polynomial-time algorithm.

We consider a new pricing model that are designed for the study of competitive pricing. This model are generalization of the problem studied in [1, 2]. The proposed model can be described as Stackelberg leader–competitor–clients game. There are two sets of facilities: a set of leader's facilities and a set of competitor's facilities. Also we have a set of clients. Each client has a budget and a demand. First the leader assigns price. After that, the competitor assigns price. The players compete for client's demand. Each client knows the transportation cost of servicing each facility. He selects a facility with minimal total payment (price and transportation cost) and buys the product if his payment does not exceed his budget. In this game need to set the leader's price in order to maximize overall revenue of the leader.

The model is formulated as a three–level linear programming problem with integer and boolean variables. It is shown that if clients cooperate with the leader and the players use uniform pricing then there is an exact polynomial-time algorithm for solving the three-level problem. The same result was obtained for the case when clients cooperate with the competitor.

This research was supported by RFBR grant 16-07-00319.

References

[1] Panin A., Plyasunov A. (2013) The pricing problem. Part I: Exact and approximate algorithms. *Journal of Applied and Industrial Mathematics*, Vol. 7, Issue 2, pp. 241–251.

[2] Panin A., Plyasunov A. (2013) The pricing problem. Part II: Computational complexity. *Journal of Applied and Industrial Mathematics*, Vol. 7, Issue 3, pp. 420–430.

Special Session

"Numerical and Computational Methods in Data Analysis and Classification"

Organizers:

Gerardo Toraldo

Salvatore Cuomo

University of Naples Federico II, Italy

Computational issues in Linear Multistep Method Particle Filtering

Daniela Calvetti, Erkki Sommersalo

Department of Mathematics, Case Western Reserve University
10900 Euclid Ave., Cleveland, OH 44106, USA

Salvatore Cuomo, Monica Pragliola, Gerardo Toraldo

Department of Mathematics, University of Naples Federico II
Via Cintia 21, 80126, Naples, Italy

Keywords. Inverse Problems, Sampling Techniques, Particle Filtering, Linear Multistep Methods.

The Linear Multistep Method Particle Filter (LMM PF) is a method for predicting the evolution in time of a evolutionary system governed by a system of differential equations. If some of the parameters of the governing equations are unknowns, it is possible to organize the calculations so as to estimate them while following the evolution of the system in time. The underlying assumption in the approach that we present is that all unknowns are modelled as random variables, where the randomness is an indication of the uncertainty of their values rather than an intrinsic property of the quantities. Consequently, the states of the system and the parameters are described in probabilistic terms by their density, often in the form of representative samples. This approach is particularly attractive in the context of parameter estimation inverse problems, because the statistical formulation naturally provides a means of assessing the uncertainty in the solution via the spread of the distribution. The computational efficiency of the underlying sampling technique is crucial for the success of the method, because the accuracy of the solution depends on the ability to produce representative samples from the distribution of the unknown parameters. The LMM PF algorithm was originally proposed in [1]. In this paper LMM PF is tested on a skeletal muscle metabolism [2] problem, which was previously treated within the Ensemble Kalman filtering framework. Here numerical evidences are used to highlight the correlation between the main sources of errors and the influence of the linera multistep method adopted. Finally, we analyzed the effect of replacing LMM with Runge-Kutta class integration methods for supporting the PF technique.

References

[1] Arnold A, Calvetti D and Somersalo E 2013 *Linear multistep methods, particle filtering and sequential Monte Carlo* Inverse Problems **29** 085007.

[2] Arnold A, Calvetti D and Somersalo E 2014 *Parameter estimation for stiff deterministic dynamical systems via ensemble Kalman filter*, Inverse Problems **30** 105008

A second order derivative scheme for the Bregman Algorithm class

Rosanna Campagna, Serena Crisci, Salvatore Cuomo, Ardelio Galletti, Livia Marcellino

University of Naples Federico II, Department of Mathematics and Applications, Italy
University of Naples Federico II, Department of Mathematics and Applications, Italy
University of Naples Federico II, Department of Mathematics and Applications, Italy
University of Naples Parthenope, Department of Science and Technology, Italy
University of Naples Parthenope, Department of Science and Technology, Italy
rosanna.campagna@unina.it, se.crisci@studenti.unina.it,
salvatore.cuomo@unina.it, ardelio.galletti@uniparthenope.it,
livia.marcellino@uniparthenope.it

Keywords. Split Bregman Method; MRI Denoising; Iterative Methods.

The algorithms based on Bregman iterative regularization are known because of their efficiency for convex constraint optimization problems. In this paper, we introduce a second order derivative scheme for the class of Bregman Algorithms. Particularly its properties of convergence and stability for regularization with a "Hessian-like" penalty term are investigated. Moreover, we apply the proposed scheme to an isotropic Total Variation (TV) problem arising in Magnetic Resonance Image (MRI) denoising. This represents a recent trend in MRI research field related to design and adoption of algorithms that are able to denoise and reconstruct clinical data in a reliable way. Experimental results confirm that our algorithm has good performance in terms of reconstruction quality, effectiveness and robustness, compared with some other frequently used methods for the image reconstruction.

References

[1] Goldstein T. and Osher S. (2009) The Split Bregman Method for $L1-$Regularized Problems. *SIAM J. Img. Sci.* Vol. 2, Issue 2, pp. 323–343.

[2] Bregman L. M. (1967) The Relaxation Method of Finding Common Point of Convex Sets and its Application to the Solution of Problems in Convex Programming, *Computational Mathematics and Mathematical Physics*, Vol. 7, no. 3, pp. 200–217.

[3] Cuomo S., De Michele P. and Piccialli F. (2014) 3D data denoising via Nonlocal means filter by using parallel GPU strategies. *Computational and Mathematical Methods in Medicine*, Vol. 2014

[4] Piccialli F., Cuomo S. and De Michele P. (2013) A Regularized MRI Image Reconstruction based on Hessian Penalty Term on CPU/GPU Systems, *Procedia Computer Science, 2013 International Conference on Computational Science*, vol. 18, pp. 2643–2646.

Scaled first-order methods for a class of large-scale constrained least squares problems

Vanna Lisa Coli, Valeria Ruggiero, Luca Zanni

University of Modena and Reggio Emilia, Via Campi 213/B, Modena, Italy
University of Ferrara, Via Saragat 1, Ferrara, Italy
vannalisa.coli@unimore.it, valeria.ruggiero@unife.it,
luca.zanni@unimore.it

Keywords. Forward-backward methods; Acceleration techniques; Diffusion MRI.

Many inverse problems arising in signal and imaging restoration can be reduced to the numerical solution of a class of large-scale constrained least squares problems, where the $M \times N$ matrix A of the objective function has nonnegative entries and theconstraints are such that the projection of a vector onto the feasible region can be performed by means of non-expensive $O(N)$ algorithms.

Significant examples of such feasible regions are provided by bound or box constraints or their combination with a single linear equality/inequality. We also assume that the size N of the problem is very large, $M << N$ and only the operators performing the matrix-vector products involving A and A^T are available. These assumptions, satisfied for example in many variational formulations of large-scale imaging problems, make some popular state-of-the-art approaches based on the availability of the matrix A in memory not convenient or inapplicable. Conversely, general forward–backward schemes exploiting only the objective gradient and the projection onto the feasible region appear very promising. Indeed, the convergence rate of these methods can be improved by means of different strategies that impact on the key components of the iterate, such as the step-length selection rules [4], the extrapolation/inertial techniques [2] or the projection/proximal steps with respect to variable metrics [3].

Starting from very recent advances on these acceleration ideas, we propose metrics tailored for the considered problems that combine well with state-of-the-art step-length selection rules and extrapolation techniques. The convergence rate improvements due to the proposed scaled first-order schemes are evaluated on both randomly generated test problems and real data arising from a problem of fibre orientation estimation in diffusion MRI [1].

References

[1] Auría A. et al. (2015) Structured sparsity for spatially coherent fibre orientation estimation in diffusion MRI. Neuroimage **115**, 245-255.
[2] Beck A., Teboulle M. (2009) A fast iterative shrinkage-thresholding algorithm for linear inverse problems. SIAM J. Imaging Sci. **2(1)**, 183-202.
[3] Bonettini S., Porta F., Ruggiero V.: A variable metric inertial method for convex optimization. Submitted, arXiv:1506.02900.
[4] Porta F., Prato M., Zanni L. (2015) A new steplength selection for scaled gradient methods with application to image deblurring J. Sci. Comp., **65**, 895–919.

Using Smooth Approximations of the Zero-Norm for Cluster Analysis

Andrea Cristofari, Alberto De Santis, Stefano Lucidi

Department of Computer, Control, and Management Engineering, Sapienza University of Rome, Via Ariosto, 25, 00185 Rome, Italy
cristofari@dis.uniroma1.it,
desantis@dis.uniroma1.it,lucidi@dis.uniroma1.it

Keywords. Nonlinear programming; cluster analysis; zero-norm approximation.

Cluster analysis is one of the most widely studied topics in Machine Learning. It deals with grouping objects on the basis of their similarity and arises in many different fields and in many real world applications. As there is no objectively "right" clustering method, many models and algorithms were studied in the last decades.

Here, we are concerned with the approach proposed in [1], in which the clustering problem is formulated as penalized regression, by minimizing a least squares term and a fusion penalty term. The idea is to introduce a centroid for each observation, representing the cluster which the sample belongs to. The problem consists in minimizing the distances between the samples and the corresponding centroids, trying at the same time to group centroids with the penalty term. The main issue of this approach is to make some pairs of centroids coincide, in order to form clusters. To this aim, weighted zero-norm penalties are employed in this work. To solve the resulting problem, the penalty term is approximated with a sequence of smooth functions that converges to the zero-norm pointwise, extending some approaches proposed in literature [2]. In this way, the approximating problems can be solved by standard algorithms for smooth optimization. Moreover, the convergence of the global minimum points of the approximating problems towards global minimum points of the original problem can be established.

This model can be applied in different contexts, both when the number of clusters is unknown and when it is fixed a priori. Numerical results on some synthetic and real data sets are provided.

References

[1] Hocking T.D., Joulin A., Bach F., and Vert J.P. (2011) Clusterpath an algorithm for clustering using convex fusion penalties. In *28th international conference on machine learning*.

[2] Mangasarian O.L. (1996) Machine learning via polyhedral concave minimization. *Applied Mathematics and Parallel Computing*, pp. 496–499.

Collaborative Reputation Systems in a Cultural Heritage Scenario

Salvatore Cuomo[1], Pasquale De Michele[1], Ardelio Galletti[2], Giovanni Ponti[3]

[1]University of Naples Federico II,
Strada Vicinale Cupa Cintia 21, 80126, Naples, Italy
[2]University of Naples Parthenope,
Centro Direzionale Isola C4, 80163, Naples Italy
[3]ENEA Research Center,
Portici, Naples, Italy
{salvatore.cuomo, pasquale.demichele}@unina.it,
ardelio.galletti@uniparthenope.it, giovanni.ponti@enea.it

Keywords. Collaborative Reputation Systems; Convergence; Iterative Methods; Cultural Heritage.

In the last decade, algorithms for reputation systems are been widely developed in order to achieve correct ratings for products, services, companies, digital contents and people. We start from the model proposed in [1], where a comprehensive mathematical model for Collaborative Reputation Systems (CRSs) is formally defined as a recurrence relation that generates a sequence of trust matrices, from which the reputation of the items and the raters can be derived. Even though our model can be applied to several scenarios, the focus of this work is related to its application in a real case, that is the *cultural event scenario* [2]. More in detail, in cultural heritage environment, the data collected in an event represent the basic knowledge to be inferred. The main idea is to correctly use the available technology and data to give a reliable rate (reputation) for both visitors and artworks. These rates will be very useful to classify the visiting style of the visitors and to fix the artworks that have most attracted visitors. Finally, the challenge is to apply the proposed mathematical model to detect common visitor behaviours, predict visiting dynamics and recommend services and tools for cultural spaces.

References

[1] Galletti, A., Giunta, G., Schmid, G.. *A mathematical model of collaborative reputation systems*. International Journal of Computer Mathematics, 89 (17), pp. 2315-2332, 2012. DOI: 10.1080/00207160.2012.715641

[2] Cuomo S., De Michele, P., Galletti, A., Ponti G.. *Visiting Styles in an Art Exhibition Supported by a Digital Fruition System*. 11th International Conference on Signal-Image Technology & Internet-Based Systems, SITIS 2015, Bangkok, Thailand, November 23-27, 2015, pp. 775-781 SITIS, 2015.

Some error bounds for K-iterated Gaussian recursive filters

Salvatore Cuomo, Ardelio Galletti, Giulio Giunta, Livia Marcellino

University of Naples Federico II
salvatore.cuomo@unina.it
University of Naples Parthenope
{ardelio.galletti,giulio.giunta,livia.marcellino}@uniparthenope.it

Keywords. Gaussian Convolution; Recursive Filtering; Error Bounds.

Recursive filters (RFs) have achieved a central role in several research fields over the last few years. For example, they are used in image processing, in data assimilation [1, 2] and in elec-trocardiogram denoising. More in particular, among RFs, the Gaussian RFs are an efficient computational tool for approximating Gaussian-based convolutions and are suitable for dig-ital image processing and applications of the scale-space theory. As is a common knowledge, the Gaussian RFs, applied to signals with support in a finite domain, generate distortions and artifacts, mostly localized at the boundaries. Heuristic and theoretical improvements have been proposed in literature [4] to deal with this issue (namely boundary conditions). They include the case in which a Gaussian RF is applied more than once, i.e. the so called K-iterated Gaussian RFs. In this paper, starting from a summary of the comprehensive mathematical background, we consider the case of the K-iterated first-order Gaussian RF and provide the study of its numerical stability and some component-wise theoretical error bounds.

References

[1] Cuomo, S., Farina, R., Galletti, A., Marcellino, L. *An error estimate of Gaussian recursive filter in 3Dvar problem.* Federated Conference on Computer Science and Information Systems, FedCSIS 2014, art. no. 6933068, pp. 587-595, 2014. DOI: 10.15439/2014F279

[2] Farina, R., Dobricic, S., Storto, A., Masina, S., Cuomo, S. *A revised scheme to compute horizontal covariances in an oceanographic 3D-VAR assimilation system*, Journal of Computational Physics, 284, pp. 631-647, 2015. DOI: 10.1016/j.jcp.2015.01.003

[3] Cuomo, S., De Pietro, G., Farina, R., Galletti, A., Sannino, G. *A novel O(n) numerical scheme for ECG signal denoising Procedia Computer Science*, 51 (1), pp. 775-784, 2015. DOI: 10.1016/j.procs.2015.05.198

[4] Cuomo, S., Farina, R., Galletti, A., Marcellino, L. *A K-iterated scheme for the first-order Gaussian Recursive Filter with boundary conditions.* Federated Conference on Computer Science and Information Systems, FedCSIS 2015, pp.641-647, 2015. DOI: 10.15439/2015F286

Nonlinear Programming for classification problems in machine learning

Manlio Gaudioso, Annabella Astorino, Antonio Fuduli

Universitá della Calabria, DIMES, Via P. Bucci, Rende (CS), Italy
ICAR-CNR, Via P. Bucci, Rende (CS), Italy
Universitá della Calabria, Dip. Mat. e Inf., Via P. Bucci, Rende (CS), Italy
manlio.gaudioso@unical.it, astorino@icar.cnr.it, antonio.fuduli@unical.it

Keywords. Classification; Machine learning; Nonsmooth optimization.

Classification is a machine learning technique aimed at assigning exactly one, from among several classes, to each sample in a population, the sample being identified as a vector of numerical values of a certain number of attributes. The classification process works as follows. Starting from a dataset of samples with known class membership, a mathematical tool is developed (the classifier) which is able to predict the class membership for any newly incoming sample. The ability to correctly classify a new sample is called the generalization capability. The field has become more and more relevant as possible applications touch a quite wide range of practical problems in areas such as text and web classification, object recognition in machine vision, gene expression profile analysis, DNA and protein analysis, medical diagnosis, customer profiling etc.

Construction of a classifier requires in general solution of a numerical optimization problem to detect an "optimal" separation surface in the space of the samples. Separation of sets has been a very important field of interest in mathematics, we just recall here the celebrated Hahn-Banach theorem. In particular, separability of two sets by means of a hyperplane is a property of the geometry of the sets connected to the notion of convex set. Thus linear separability of sets has been at the basis of the most popular approach to classification, the Support Vector Machine (SVM) model, where one looks for a hyperplane separating two given sample sets. Parallel to the development of SVM methods, the use of nonlinear separating surfaces in the dataset space, instead of hyperplanes, has received in recent years some attention. The objective of the talk is to survey such proposals, mainly in terms of the numerical optimization algorithms which are required to construct the surfaces. In particular we will consider polyhedral, ellipsoidal, spherical and conical separation approaches.

In all of them the separation process takes place in the original input space and does not require mapping to higher dimension spaces.

On the Regularization of Generalized Eigenvalues Classifiers

Mario Guarracino and Mara Sangiovanni
High Performance Computing and Networking Institute, National Research Council of Italy - Naples, Italy

Gerardo Severino
University of Naples Federico II, Division of Agricultural, Forest and Biosystems Engineering - Portici, Italy

Gerardo Toraldo
University of Naples Federico II, Department of Mathematics, Naples, Italy, toraldo@unina.it

Marco Viola
Sapienza University of Rome, Department of Computer, Control and Management Engineering - Rome, Italy

Keywords. Semisupervised classification Generalized eigenvalues classifiers Laplacian regularization

Generalized Eigenvalues Classifiers (GEC), which originated from the GEPSVM algorithm by Mangasarian, proved to be an efficient alternative to the Support Vector Machines (SVMs) in the solution of supervised classification tasks. However real-life datasets are often characterized by a large number of redundant features and by a great number of points whose labels are difficult (or too expensive) to assign. In this work we start from the Regularized Generalized Eigenvalue Classifier (ReGEC) and show how regularization terms can be used to enable the classifier to solve two different problems, strictly connected to that of supervised classification: feature selection and semi-supervised classification. Numerical results, obtained on some standard benchmark data sets, show the efficiency of the proposed solutions.

A Note on Spectral Properties of Some Gradient Methods

Gerardo Toraldo
Department of Mathematics, University of Naples Federico II, via Cintia 21, 80126, Naples, Italy, toraldo@unina.it

Daniela di Serafino
Department of Mathematics and Physics, Second University of Naples, viale A. Lincoln, 5, Caserta I-81100, Italy, daniela.diserafino@unina2.it

Valeria Ruggiero
Department of Mathematics and Computer Science, University of Ferrara, via Saragat 1, Ferrara I-44122, Italy, valeria.ruggiero@unife.it

Luca Zanni
Department of Physics, Computer Science and Mathematics, University of Modena and Reggio Emilia, via Campi 213/B, Modena I-41125, Italy, luca.zanni@unimore.it

Keywords. Nonlinear optimization, gradient methods, Hessian spectral properties

Several strategies for accelerating gradient methods have been devised in the last years, stimulated by the seminal work by Barzilai and Borwein [1]. These strategies follow the idea of defining steplengths that capture spectral properties of the Hessian of the objective function; based on them, new first-order methods for continuous nonlinear optimization have been designed, which showed to be effective in some practical contexts [2, 3]. Nevertheless, there is still a lack of satisfactory understanding of the behavior of the new methods. In this talk we present the spectral properties of some recently proposed steplength rules and some general theoretical results [4], with the aim to provide insight into the computational effectiveness and regularization properties of gradient methods. Numerical experiments supporting the theoretical analysis are reported.

References

[1] Barzilai, J., Borwein, J.M. (1988) *Two-point step size gradient methods*, IMA J. Numer. Anal., 8 (1), pp. 141-148

[2] Porta, F., Prato, M., Zanni, L.(2015) *A New Steplength Selection for Scaled Gradient Methods with Application to Image Deblurring*, J. Sci. Comput. 65 (3), pp. 895-919

[3] De Asmundis, R., di Serafino, D., Landi, G. (2016) *On the regularizing behavior of the SDA and SDC gradient methods in the solution of linear ill-posed problems*, J. of Comput. and Appl. Math., 302, pp. 81-93

[4] De Asmundis, R., di Serafino, D., Riccio, F., Toraldo, G. (2013) *On spectral properties of steepest descent methods*, IMA J. Numer. Anal., 33 (4), pp. 1416-1435

Special Session
"Numerical Global Optimization Algorithms"

Organizers:

Roman Strongin
Vladimir Grishagin
"Lobachevsky" University of Nizhni Novgorod, Russia

Local Tuning in Multilevel Scheme of Parallel Global Optimization

Konstantin Barkalov, Ilya Lebedev

University of Nizhni Novgorod, Nizhni Novgorod, Russia
barkalov@vmk.unn.ru, lebedev@vmk.unn.ru

Keywords. Global optimization; parallel computing; Peano-type space filling curves; nested optimization scheme.

This work considers a parallel algorithm for solving the multidimensional multiextremal optimization problems. The algorithm combines nested optimization scheme [1] and Peano-type space filling curves [2] for the dimensionality reduction. Such a multilevel optimization scheme allows solving the multidimensional problems by the reduction of these ones to the parallel solving of a set of the data-independent subproblems with a smaller dimensionality [3].

Some local tuning techniques for the global optimization methods have been proposed in [1, 2]. In the present study, we used one of these based on the adaptive estimation of global optimizer. Local refinement in the multilevel optimization scheme decreases the number of iterations considerably. Parallel algorithm with mixed local-global strategy of search is proposed as well.

The efficiency of the parallel algorithm was investigated on Lobachevsky supercomputer (http://www.top500.org/system/178472). The speedup of the algorithm using several nodes as compared with the serial algorithm has been demonstrated experimentally. The computational experiments were carried out on a series of several hundred multidimensional problems of well-known multiextremal test class GKLS.

Acknowledgements.

This research was supported by the Russian Science Foundation, project No 15-11-30022 "Global optimization, supercomputing computations, and applications".

References

[1] Strongin R.G., Sergeyev Ya.D. (2000) *Global optimization with non-convex constraints. Sequential and parallel algorithms.* Kluwer Academic Publishers, Dordrecht.

[2] Sergeyev Ya.D., Strongin R.G., Lera D. (2013) *Introduction to global optimization exploiting space-filling curves.* Springer.

[3] Barkalov K.A., Gergel V.P. (2014) Multilevel scheme of dimensionality reduction for parallel global search algorithms. In Proceedings of the *International Conference on Engineering and Applied Sciences Optimization* (ed. by Lagaros N.D.), Kos Island (Greece), pp. 2111–2124.

New optimization problems arising in modelling of 2D-crystal lattices

Yuri Evtushenko, Mikhail Posypkin

Dorodnicyn Computing Centre, FRC CSC RAS, Vavilov st. 40, Moscow, Russia
evt@ccas.ru, mposypkin@gmail.com

Keywords. Global optimization;Optimization methods;Crystal lattice.

Nano-technologies and material science often give rise to optimization problems. Some of them become popular benchmarks for optimization software [1]. In this paper we present new optimization problems arising in modelling of 2D-crystals.

The problem consists in finding a structure of a fragment of two-dimensional crystal lattice with the minimal energy. Atoms in a lattice reside on parallel lines (layers). The interatomic distances are the same within one layer but can differ for distinct layers. Formally the problem is stated as follows:

$$f(x) \to \min, s.t.\, a_i \le x_i \le b_i, i = 1, \ldots, n, \tag{1}$$

where $x = (h_1, d_1, s_1, \ldots, h_n, d_n, s_n)$, h_i is the distance between i-th and $(i-1)$-th layer, d_i — the displacement of the first atom in i-th layer and s_i is the interatomic distance between adjacent atoms in i-th layer. The energy $f(x)$ of the piece of material is computed using so-called potential functions. We used Lennard-Jones, Morse and Tersoff potentials. Problem (1) belongs to the class of non-differentiable box-constrained optimization problems.

The paper evaluates various optimization techniques for the problem (1), compare their performances and draws the conclusion about best choice of optimization methods and parameter selection for the problem under test. As a result we were able to locate minima meaningful from the physical point of view, e.g. reproducing graphene lattice.

Acknowledgements.

This research was supported by Russian Science Fund, project 14-11-00782.

References

[1] Wales D. J., Doye J. P. (1997) Global optimization by basin-hopping and the lowest energy structures of Lennard-Jones clusters containing up to 110 atoms. *T*he Journal of Physical Chemistry A, 101(28) pp. 5111–5116.

Accelerating Multicriterial Optimization by the Intensive Exploitation of Accumulated Search Data

Victor Gergel, Evgeny Kozinov

University of Nizhni Novgorod, Nizhni Novgorod, Russia
gergel@unn.ru, kozinov@vmk.unn.ru

Keywords. Multicriterial decision making; global optimization problems; high performance computing; computing efficiency.

The rational choice problems are widespread in the scientific and technological human activities. Such problems as the optimal arrangement of the elements of the integrated circuits, aircraft design, medical drug development, etc. can serve as the examples of the applied problems, which the choice of the rational solutions is necessary in (see, for example, [1]). All the problems mentioned above can be represented as the global optimization ones [2]. It is worth noting that the above problems are the multiple criterial ones, as a rule.

For solving the multiple criteria problems, it is necessary to apply the algorithms utilizing efficiently all the computation resources available [3]. In [1, 2, 3] the information-statistical approach has been applied. All the information on the object of investigation accumulated in the search process is utilized in finding the the optimized solution. The methods for reuse of the accumulated information when altering the problem statement are considered in the article.The reuse of the accumulated information allows managing the search process and increasing the efficiency of solving the problems when altering the search parameters. The approach proposed is illustrated by an example of the developed demonstration system.

References

[1] Gergel, V., et al. (2013) High Performance Computing in Biomedical Applications. *Procedia Computer Science*, Vol. 18, pp. 10–19.

[2] Strongin R.G., Sergeyev Ya.D. (2000) Global optimization with non-convex constraints. Sequential and parallel algorithms. *Kluwer Academic Publishers, Dordrecht.*

[3] Strongin R.G., Gergel V.P. (2003) Parallel computing for globally optimal decision making *Lecture Notes in Computer Science* Vol. 2763, pp. 76–88.

Optimization Problems in Structured Low Rank Approximation

Jonathan Gillard

Cardiff School of Mathematics, Cardiff University, UK
GillardJW@Cardiff.ac.uk, ZhigljavskyAA@Cardiff.ac.uk

Keywords. Low rank approximation; Global optimization; Time series analysis.

In this talk we illustrate some optimization challenges in the structured low rank approximation (SLRA) problem. SLRA can be described as the problem of finding a low rank approximation of an observed matrix which has the same structure as this matrix (such as Hankel). We demonstrate that the optimization problem arising is typically very difficult: in particular, the objective function is multiextremal even for simple cases.

The main theme of the talk is to suggest that the difficulties described in approximating a solution of the SLRA problem open huge possibilities for the application of stochastic methods of optimization. A traditional method of approximating the solution of the Hankel SLRA problem are the so-called Cadzow iterations, which consist of alternating projections between the space of low rank matrices (obtained via the singular value decomposition) and the space of Hankel matrices (by averaging over the anti-diagonals). Cadzow iterations are known to behave poorly; despite Cadzow's initial claim that it is a globally convergent algorithm, this algorithm is not even locally convergent.

We will also describe some issues in low rank approximation when we wish to weight each of our observations.

Acknowledgements. The speaker would like to acknowledge and thank his collaborators on this topic: Dr Dmitri Kvasov and Prof Anatoly Zhigljavsky.

References

[1] Gillard, J. W. and Kvasov, D. E. (2016). Lipschitz optimization methods for fitting a sum of damped sinusoids to a series of observations. *Statistics and Its Interface*, to appear.

[2] Gillard, J. W. and Zhiglavsky, A. A. (2015). Stochastic algorithms for solving structured low-rank approximation problems. *Communications in Nonlinear Science and Numerical Simulation*, Vol. 21(1-3), pp. 70–88.

[3] Gillard, J. W. and Zhigljavsky, A. A. (2012). Optimization Challenges in the Structured Low Rank Approximation Problem. *Journal of Global Optimization*, Vol. 57(3), pp. 733–751.

[4] Gillard, J. W. and Zhigljavsky, A. A. (2011). Analysis of structured low rank approximation as an optimisation problem. *Informatika*, Vol. 22(4), pp. 489-505.

On global optimization using an estimate of Lipschitz constant and simplicial partition

Albertas Gimbutas, Antanas Žilinskas

Vilnius University, Akademijos str. 4, LT-08663 Vilnius, Lithuania
albertas.gimbutas@mii.vu.lt, antanas.zilinskas@mii.vu.lt

Keywords. Lipschitz optimization; global optimization; simplicial partition

An algorithm is proposed for finding the global minimum of a multi-variate black-box Lipschitz function with an unknown Lipschitz constant. The feasible region is initially partitioned into simplices; in the subsequent iteration, the most suitable simplices are selected and bisected via middle point of the longest edge. The suitability of a simplex for bisection is evaluated by minimization over that simplex of a surrogate function which mimics the lower bound for the considered objective function. The surrogate function is defined almost identically with the Lipschitz lower bound but an estimate is used instead of the true Lipschitz constant. The proposed algorithm is similar to those described in [1]; the novelty of the algorithm is in the sophisticated method of estimating the Lipschitz constant, and in the appropriate method of minimization of the surrogate function.

The proposed algorithm was tested using the well-known test problems, as well as random test problems generated using the generator presented in [2]. The numerical results show that the proposed algorithm finds the global minimizer with the prescribed accuracy spending a smaller number of function evaluations, however it requires more computing time for auxiliary computations than other DIRECT type algorithms.

References

[1] Paulavičius R., Žilinskas J. (2014) Simplicial Lipschitz optimization without the Lipschitz constant. *Journal of Global Optimization*, Vol. 59, No. 1, pp. 23–40.

[2] Gaviano M., Kvasov D.E., Lera D., Sergeyev Y.D. (2003) Algorithm 829: Software for generation of classes of test functions with known local and global minima for global optimization. *ACM Transactions on Mathematical Software (TOMS)*, Vol. 29, No. 4, pp. 469–480.

Clustering-based statistical global optimization

Gražina Gimbutienė, Antanas Žilinskas

Vilnius University, Akademijos 4, LT-08663 Vilnius, Lithuania
grazina.gimbutiene@mii.vu.lt, antanas.zilinskas@mii.vu.lt

Keywords. global optimization; statistical models; clustering.

The global optimization problem $\min_{x \in A} f(x)$ of expensive black-box objective functions over a hyper-rectangle $A \subset R^d$, $A = [a_i, b_i], i = 1, \ldots, d$, is considered. Due to the uncertainty inherent in such formulation of the problem, a rational optimizer needs a statistical model to support the choice of the function evaluation sequence. The original versions of the algorithms based on statistical models of the objective function were proved to possess the property of average optimality, however, they involve non-trivial auxiliary optimization of statistical criteria over A at each iteration. Therefore extensions to these algorithms are crucial to expand their usage to less expensive objective functions.

An example is the original version of the so-called P-algorithm, which, given the already known observations $x_i, y_i = f(x_i), i = 1, \ldots, n$, maximizes the probability of improvement, in order to select the next function evaluation location:

$$x_{n+1} = \arg\max_{x \in A} P(\xi(x) < y_{on} - \epsilon_n | x_i, y_i, i = 1, \ldots, n), \tag{1}$$

where $\xi(x)$ is the unknown objective value at $x \in A$, $y_{on} = \min\{y_i, i = 1, \ldots, n\}$ and $\epsilon_n > 0$ is a parameter sequence. The problem (1) might itself be multi-modal, although it is not obligatory to solve it precisely to continue the optimization process. The approach taken in recent extensions to the P-algorithm includes the rectangular decomposition of A to break (1) down into a set of smaller optimization problems over sub-regions of A. A local statistical model of f over a hyper-rectangle is employed, based on the values of the function at its vertices.

We pursue the similar line of reasoning in this work. However, the goal of modeling the objective function is to make a compromise between the available information over isolated hyper-rectangles and their clusters, possibly corresponding to local minima, and thus increase the convergence speed of the resulting algorithm. Therefore clusters of hyper-rectangular subsets of A are formed and homogeneous isotropic Gaussian random fields are used to model the objective function over them. All generated hyper-rectangles are ranked by the statistical criterion value, e. g. the analogue to the improvement probability, computed at the locations that might be used to subdivide them, and the best hyper-rectangle is partitioned. Numerical experiments are performed to demonstrate the advantages of the proposed approach.

Acknowledgements.

This work was supported by the Research Council of Lithuania under Grant No. MIP-051/2014.

Comparative efficiency of dimensionality reduction schemes in global optimization

Vladimir Grishagin, Ruslan Israfilov, Yaroslav Sergeyev

Department of Software and Supercomputing, Lobachevsky State University of Nizhni Novgorod, Russia
vagris@unn.ru, ruslan@israfilov.com, yaro@dimes.unical.it

Keywords. Global optimization; dimensionality reduction; nested optimization schemes; space-filling curves; operation characteristics.

The multidimensional global optimization problem

$$\min\{f(y): y \in Q\},\ Q = \{y \in \mathbb{R}^N: a_i \le y_i \le b_i, 1 \le i \le N\} \qquad (1)$$

is considered, where Q is a hyperinterval in the Euclidean space $\mathbb{R}^N$.

For multiextremal problems (1) the dimension is a crucial factor influencing significantly on their computational complexity. There are several approaches which apply ideas of dimensionality reduction for the development of efficient global optimization algorithms, for example, schemes of nested optimization reducing the initial problem (1) to a family of subproblems with lesser dimensions [1, 2] or techniques of mapping the multidimensional search domain Q onto unit interval in by means of Peano-type space-filling curves [1, 3].

In this paper we present the results of experimental comparison for several global optimization methods based on approaches mentioned above in combination with characteristical algorithms solving subproblems of lesser dimensions under the assumption that the objective function $f(y)$ in the domain Q satisfies the Lipschitz condition. The experiments were executed on widely used test multiextremal classes of different dimensions. For comparison of the investigated algorithms the method of operation characteristics [2] was used as a tool of demonstrable evaluation of the efficiency.

Acknowledgements.

This research was supported by the Russian Science Foundation, project No 15-11-30022 "Global optimization, supercomputing computations, and applications".

References

[1] Strongin R.G., Sergeyev Ya.D. (2000) *Global optimization with non-convex constraints. Sequential and parallel algorithms.* Kluwer Academic Publishers, Dordrecht.

[2] Gergel V., Grishagin V., Gergel A. (2015) Adaptive nested optimization scheme for multidimensional global search. *Journal of Global Optimization*, pp. 1–17.

[3] Sergeyev Ya.D, Strongin R.G., Lera D. (2013) *Introduction to Global Optimization Exploiting Space-Filling Curves.* Springer, New York.

One Approach to Fractional Programming via D.C. Optimization Problems

Tatiana Gruzdeva, Alexander Strekalovskiy

Matrosov Institute for System Dynamics and Control Theory of SB RAS,
Lermontov str., 134, Irkutsk, Russia
gruzdeva@icc.ru, strekal@icc.ru

Keywords. Nonlinear fractional programs; global optimization; nonconvex quadratic programming problems; local search algorithms.

Our research is devoted to development of efficient global search methods for sum of ratios fractional programming problem [1]:

$$(\mathcal{P}) \qquad f(x) := \sum_{i=1}^{m} \frac{\psi_i(x)}{\phi_i(x)} \downarrow \min_x, \quad x \in S.$$

This is a nonconvex problem with multiple local extremum which belongs to a class of global optimization.

We proved the reduction (equivalence) theorem for the fractional programming problem with the d.c. functions and the solution of the equation with the vector parameter of the sum of d.c. functions that satisfy the nonnegativity assumption. This theorem opens the door to a justified use of the Dinkelbach's algorithm in solving fractional programming problems where the goal function is a sum of fractions given by d.c. functions.

Also we investigated the well-known equivalent statement of the fractional programming problem [2] with the d.c. functions in the form of the minimization of the linear function over a non-convex set defined via the d.c. inequality constraints. Based on the global optimality conditions for problems with d.c. constraints, we developed the local search method and tested it on the fractional programming problems where the summable fractions are given by linear and/or convex quadratic functions. The testing was carried out on a specially designed set of test examples.

Acknowledgements. This research was supported by the Russian Science Foundation (project No. 15-11-20015).

References

[1] J. B. G. Frenk, S. Schaible (2002) Fractional Programming. In Handbook of Generalized Convexity and Generalized Monotonicity (ed. by N. Hadjisavvas, S. Komlosi, S. Schaible), Series Nonconvex Optimization and Its Applications, V. 76, Springer, pp. 335–386.

[2] M. Dur, R. Horst, N.V. Thoai (2001) Solving sum-of-ratios fractional programs using efficient points *Optimization*, Vol. 49, pp. 447–466.

Remarks on global optimization using space-filling curves

Daniela Lera, Yaroslav Sergeyev

Dipartimento di Matematica e Informatica, University of Cagliari, Italy.
Dipartimento di Ingegneria Informatica, Modellistica, Elettronica e Sistemistica,
Univ. of Calabria, Italy - Lobachevsky State Univ. of Nizhni Novgorod, Russia
lera@unica.it, yaro@dimes.unical.it

Keywords. Global Optimization; space-filling curves approximations; Lipschitz constant.

In this paper, the global optimization problem: $\min_{y \in S} F(y)$ with S being a hyperinterval in R^N and $F(y)$ satisfying the Lipschitz condition with an unknown Lipschitz constant is considered. It is supposed that the function $F(y)$ can be multiextremal, non-differentiable, and given as a "black-box". To attack the problem we consider the following two ideas. First, an approach that uses numerical approximations of space-filling curves to reduce the original Lipschitz multi-dimensional problem to a univariate one satisfying the Hölder condition [1, 2]. Second, we propose different techniques for acquiring the Hölder information that can be distinguished with respect to the way the Hölder constant is estimated during the process of optimization. In particular, we consider techniques that use either a global estimate of the Hölder constant valid for the whole search region, or local estimates H_i valid only for some subregions of the domain [3]. Moreover, a new geometric technique working with a number of possible Hölder constants chosen from a set of values varying from zero to infinity showing so that ideas introduced in a popular DIRECT method can be used in the Hölder global optimization [4].

Acknowledgements. The research of Ya.D. Sergeyev was supported by the Russian Science Foundation, project No 15-11-30022 "Global optimization, supercomputing computations, and applications".

References

[1] Sergeyev Ya.D, Strongin R.G., Lera D. (2013) *Introduction to Global Optimization Exploiting Space-Filling Curves*. Springer, New York.

[2] Lera D., Sergeyev, Ya.D. (2013) Acceleration of univariate global optimization algorithms working with Lipschitz functions and Lipschitz first derivatives. *SIAM J. Optim.*, Vol. 23(1), pp. 508–529.

[3] Lera D., Sergeyev Ya.D. (2010) Lipschitz and Hölder global optimization using space-filling curves. *Applied Numerical Mathematics* Vol. 60(1-2), pp. 115–129.

[4] Lera D., Sergeyev Ya.D. (2015) Deterministic global optimization using space-filling curves and multiple estimates of Lipschitz and Hölder constants. *Commun Nonlinear Sci and Numer Simulat* Vol. 23, pp. 328–342.

Examining the Bernstein global optimization approach to optimal power flow problem

Bhagyesh V. Patil, L. P. M. I. Sampath, Ashok Krishnan,
K. V. Ling, H. B. Gooi

Cambridge Centre for Advanced Research in Energy Efficiency in Singapore, Singapore
Interdisciplinary Graduate School, Singapore
School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore
bhagyesh.patil@gmail.com
(mohashai001,ashok004,ekvling,ehbgooi)@ntu.edu.sg

Keywords. Bernstein polynomials, Convex relaxations, Global optimization, Optimal power flow.

The optimal power flow (OPF) problem is a well established area of research in the power systems community. Several solution approaches, such as sequential linear programming and interior-point methods have been investigated in the literature [1]. However, it is noteworthy that the OPF problem is nonconvex in nature and multiple number of local optima exist for the OPF problem. As such, the above mentioned solution approaches, which typically rely on a generalized convexity assumption of the optimization problem, may have a limited scope in practice.

In the present work, we introduce a global optimization procedure which is new in the context of OPF problems. This procedure is based on the well-known Bernstein form of polynomials, and uses several attractive *geometrical* properties associated with this Bernstein form [2]. The present work demonstrates the applicability of one such Bernstein global optimization algorithm in solving the OPF problem for a 3-bus power system and compares the findings with existing solution approaches.

Acknowledgements. This work was supported by the Singapore National Research Foundation (NRF) under its Campus for Research Excellence and Technological Enterprise (CREATE) programme, and Cambridge Centre for Advanced Research in Energy Efficiency in Singapore (CARES).

References

[1] F. Capitanescu, "Critical review of recent advances and further developments needed in AC optimal power flow," *Electric Power Systems Research*, vol. 136, pp. 57–68, 2016.

[2] B. V. Patil, P. S. V. Nataraj, and S. Bhartiya, "Global optimization of mixed-integer nonlinear (polynomial) programming problems: the Bernstein polynomial approach," *Computing*, vol. 94, no. 2-4, pp. 325–343, 2012.

GFS-algorithm based on simple Monte Carlo trials for solving global optimization problems

Yuri S. Popkov, Boris S. Darkhovskiy, Alexey Yu. Popkov

Institute for Systems Analysis of Russian Academy of Sciences, Moscow, Russia
Institute of Physics and Technology (State University), Moscow, Russia
National Research University "Higher School of Economics", Moscow, Russia
popkov@isa.ru, darbor2004@mail.ru, apopkov@isa.ru

Keywords. Global optimization; Monte Carlo method; Batch iterations; Sequences of "quasi-global" minima.

It is proposed a new method for solution of global optimization (GO) problems on compact sets, preset by list of inequalities. The goal function satisfies the Hölder condition with unknown constants.

The algorithm generates a batch of independent random vectors uniformly distributed on the unit multidimensional cube ((G)eneration phase). The vectors from the batch are examined to belong to the feasible set ((F)iltration phase) and a batch of feasible vectors is constructed. Then, on a final phase minimum ("quasi-global") of the goal function are (S)elected. Transition to a next iteration lies in constructing the larger batch of random vectors using some rule.

Solution of the problem is the set of found "quasi-minimal" value of the goal function, estimates of the neighborhood of exact global minimum and probability of hit in this neighborhood.

The novelty and potential efficiency of the GFS-algorithm consists in orientation towards general global optimization problems with goal functions meeting the Hölder condition with unknown constants; using batch iterations with simple Monte Carlo trials for constructing the sequence of "quasi-global" minima; definition of a probabilistic stopping-rule with estimation of neighbourhood of exact solution. Workability of the method has been approved on various tests.

Acknowledgements. This work was supported by the Russian Foundation for Basic Research (project no. 16-07-00743)

References

[1] Strongin R.G., Sergeyev Ya.D. *Global Optimization with Non-Convex Constraints. Sequential and Parallel Algorithms.* Kluwer Academic Publishers, Dordrecht, 2000.

[2] Zhigliavsky A., Žilinskas A. *Stochastic Global Optimization.* Springer, 2006.

[3] Darkhovskii B.S., Popkov A.Y., Popkov Y.S. *Monte Carlo Method of Batch Iterations: Probabilistic Characteristics* // Automation and Remote Control, 2015, Vol. 76, No. 5, pp. 776-785.

Exact Penalization for Constrained Optimization

Alexander Strekalovskiy

Matrosov Institute for System Dynamics and Control Theory of SB RAS,
Lermontov str., 134, Irkutsk, Russia
strekal@icc.ru

Keywords. Exact penalty; non-convex problems; global search theory.

In the middle of 1960s I.Eremin and W.I. Zangwill introduced a notion of exact penalization for use in the development of algorithms for nonlinear constrained optimization. Since that time, exact penalty functions play a key role in the theory of mathematical programming and a lot of specialists successfully extended the classical results and developed the foundations of the theory and algorithms of exact penalty for constrained optimization in an elegant and straightforward way.

On the other hand, as well-known, the optimization problems must be separated into two parts. The first one is a tractable case of convex problems which are numerically solvable under minimal computability assumptions. It means that the computational efforts to solve the problem at a given accuracy grow moderately with the problems dimension. In contrast to this, real-life non-convex problems are too difficult for numerical solution because of numerous (even a huge!) local and stationary points, from which contemporary optimization methods (SQP, IPM, TRM, etc.) turn out to be unable to escape. Therefore, nowadays there are (at least) two classes of techniques to globalize local algorithms: line-search and trust-region, when the progress made from x^k to x^{k+1} is measured by an auxiliary (merit, penalty) function which take into account the two contradictory goals (minimizing an objective and satisfying the constraints).

Note, however, that if the original problem was non-convex, the auxiliary one stays the same, and, therefore, the line-search, for instance, turns out to be inoperative to jump out a local pit. We propose another way to solve the penalized non-convex problems by means of Global Search Theory based on Global Optimality Conditions (GOC).

For this end we establish, first, relations between the original non-convex problem with d.c. inequality constraints and an auxiliary problem. As usually, GOC possess the so-called constructive property allowing to escape a local pit improving the value of the goal function. In addition, GOC reduce the auxiliary problem to the solving the family of convex linearized problems. The latter property leads to a Special Local Search Method the convergence of which is also investigated. The first numerical testing on a number of test problems looks rather promising.

Acknowledgements.

This research was supported by the Russian Science Foundation (project No. 15-11-20015).

One Approach for Parallel Solving a Set of Global Optimization Problems

Roman Strongin, Konstantin Barkalov

University of Nizhni Novgorod, Nizhni Novgorod, Russia
strongin@unn.ru, barkalov@vmk.unn.ru

Keywords. Global optimization; parallel computing; non-convex constraints; Peano-type space filling curves.

An efficient parallel algorithm for solving global optimization problems has been developed in University of Nizhni Novgorod [1, 2, 3, 4].

This paper suggests a new approach to parallel solving a set of global optimization problems on multiprocessor computing system. A method for adaptive balancing of computational load of processors has been investigated. Theoretical conditions that guarantee convergence to globally optimal solutions of all problems in the set have been proposed.

References

[1] Strongin R.G., Sergeyev Ya.D. (2000) *Global optimization with non-convex constraints. Sequential and parallel algorithms.* Kluwer Academic Publishers, Dordrecht.

[2] Barkalov, K.A., Strongin, R.G. (2002) A global optimization technique with an adaptive order of checking for constraints. *Computational Mathematics and Mathematical Physics*, Vol. 42(9), pp. 1289–1300.

[3] Gergel, V.P., Strongin, R.G. (2005) Parallel computing for globally optimal decision making on cluster systems. *Future Generation Computer Systems*, Vol. 21(5), pp. 673–678.

[4] Sergeyev Ya.D., Strongin R.G., Lera D. (2013) *Introduction to global optimization exploiting space-filling curves.* Springer.

A new diagonal partition-based method for global optimization problems

Julius Žilinskas[1], Remigijus Paulavičius[1], Lakhdar Chiter[2]

[1]Vilnius University Institute of Mathematics and Informatics, Akademijos 4, LT-08663 Vilnius, Lithuania
[2]Laboratoire de Mathématiques Fondamentales et Numériques, Universitéde Sétif, Sétif 19000, Algérie
julius.zilinskas@mii.vu.lt, remigijus.paulavicius@mii.vu.lt, lchiter@univ-setif.dz

Keywords. Global optimization; Lipschitz optimization; diagonal approach; bisection partitioning

We consider a global optimization problem for Lipschitz-continuous functions with an unknown Lipschitz constant. Our approach is based on the well-known DIRECT (DIviding RECTangles) algorithm [1] and motivated by a diagonal partition strategy [2]. One of the main advantages of the diagonal partitioning scheme [2] is that the objective function is evaluated at two points at each hyper-interval and therefore more complete information about the objective function is considered than using the central-sampling strategy based DIRECT algorithm. In order to efficiently use all sampling points without the objective function reevaluation authors in [2] store them in a special vertex database and retrieve it when this is necessary.

In the present talk we introduce a new DIRECT-type algorithm where sampling is performed at two diagonal points equidistant to diagonal vertices. This sampling strategy enables reuse of sampling points in bisection instead of trisection which is common for diagonal-based and DIRECT-type algorithms. The bisection is preferable to the trisection because of the shapes of hyper-intervals. Moreover, since the reuse is only in descendant hyper-intervals the database for sampled points is not needed what saves memory space and access times. The developed algorithm gives very competitive numerical results compared to the DIRECT algorithm and its well know modifications.

References

[1] Jones, D. R., Perttunen, C. D., Stuckman, B. E. (1993) Lipschitzian optimization without the Lipschitz constant. *Journal of Optimization Theory and Application*, Vol. 79 (1), pp. 157–181.

[2] Sergeyev, Y. D., Kvasov, D. E. (2006). Global Search Based on Efficient Diagonal Partitions and a Set of Lipschitz Constants. *SIAM Journal on Optimization*, Vol. 16 (3), pp. 910-937.

Regular Presentations

Optimization of Seasonal ARIMA Models Using Differential Evolution - Simulated Annealing (DESA) Algorithm in Forecasting Dengue Cases in Baguio City

Rizavel C. Addawe, Joel M. Addawe and Joselito C. Magadia

Department of Mathematics and Computer Science, College of Science, University of the Philippines Baguio, Baguio City, Philippines
School of Statistics, University of the Philippines Diliman, Quezon City, Philippines
rcaddawe@up.edu.ph, jmaddawe@up.edu.ph, jcmagadia@up.edu.ph

Keywords. ARIMA; Differential Evolution; Simulated Annealing

Accurate forecasting of dengue cases would significantly improve epidemic prevention and control capabilities. This paper attempts to provide useful models in forecasting dengue epidemic specific to the young and adult population of Baguio City. To capture the seasonal variations in dengue incidence, this paper develops a robust modeling approach to identify and estimate seasonal autoregressive integrated moving average (SARIMA) models in the presence of additive outliers. Since the least squares estimators are not robust in the presence of outliers, we suggest a robust estimation based on winsorized and reweighted least squares estimators. A hybrid algorithm, Differential Evolution - Simulated Annealing (DESA), is used to identify and estimate the parameters of the optimal SARIMA model. The method is applied to the monthly reported dengue cases in Baguio City, Philippines.

References

[1] S. Das and P. N. Suganthan, IEEE Transanctions on Evolutionary Computation **15**, 431 (2011).
[2] F. M. Tseng and G. Tzeng, Fuzzy Sets and Systems **126**, 367376 (2002).
[3] R. Addawe and J. Magadia, "Differential evolution-simulated annealing (DESA) algorithm for fitting autoregressive models to data," in *OPT-i 2014 International Conference on Engineering and Applied Sciences Optimization, Proceedings*, edited by M. Papadrakakis, M. Karlaftis, and N. Lagaros (National Technical University, Kos Island, Greece, 2014), pp. 434451
[4] R. Addawe, E. Adorio, J. Addawe, and J. Magadia, "Desa: A hybrid optimization algorithm for high dimensional functions," in *Proceedings of the Eight IASTED International Conference on Control and Applications* (ACTA Press, Montreal, QC; Canada, 2006), pp. 316321.

Implicit and Explicit Parallel Algorithms for Simulating 3D Oil Recovery problem

Darkhan Akhmed-Zaki, Timur Imankulov, Bazargul Matkerim, Beimbet Daribayev

al-Farabi Kazakh National University, al-Farabi ave.,71, Kazakhstan
darhan_a@mail.ru, imankulov.timur@gmail.com, bazargulmm@gmail.com, beimbet.daribaev@gmail.com

Keywords. MPI; CUDA; EOR; polymer; surfactant; heat transfer.

Computer technology and high-performance systems are the fastest-growing industry in the world. Therefore, the new technology give us the opportunity to solve complex problems in engineering research more efficiency. One of major problem in this area is mathematical and computer simulation of oil reservoirs. The hydrodynamic models are developing and the physical and chemical properties of underground fluids are investigating in far more detail every year. Consequently, the urgent tasks of usage of parallel algorithm for solving problems in the oil industry are growing continuously.

In this paper the three-dimensional oil displacement problem is considered, which uses chemical EOR method. The mathematical description of the problem was given by system of equations, which consists of continuity equations of the oil and water phase and the transport equations of polymer, surfactant and heat. We considered two typical schemes explicit and implicit schemes for presented 3D problem. The parallel implementations of these two schemes are realized using MPI and CUDA technologies. The parallel algorithm was tested on GPU Tesla K20 processor and supercomputer TCluster of al-Farabi KazNU.

The results of the numerical investigation on three-dimensional domain are presented and distributions of main parameters are determined. To assess the quality of the parallel algorithm calculated the speedup and efficiency for different number of processes and different mesh sizes on supercomputer.

References

[1] Danaev N., Akhmed-Zaki D., Mukhambetzhanov S., Imankulov T. (2015) Mathematical Modelling of Oil Recovery By Polymer/Surfactant Flooding. *Communications in Computer and Information Science*, Vol. 549, pp. 1–12.

[2] Akhmed-Zaki D., Mansurova M., Matkerim B., Imankulov T., Dadykina E. (2015) Development of a Distributed Parallel Algorithm of 3D Hydrodynamic Calculation of Oil Production on the Basis of MapReduce Hadoop and MPI Technologies. *Lecture Notes in Computer Science*, Vol. 9251, pp. 498–504.

[3] *nVidia CUDA* – http://www.nvidia.com/object/cuda_home_new.html.

[4] *T-cluster web site* – http://cluster.kaznu.kz/ganglia/.

Canonical Finite Element Method For Solving Nonconvex Variational Problems to Post Buckling Beam Problem

Elaf Jaafar Ali, David Yang Gao

School of Applied Science,
Federation University Australia, Mt Helen, Victoria 3353, Australia
eymath10@yahoo.com, d.gao@federation.edu.au

Keywords. Global optimization; Nonconvex variational problems; Large Deformation Elastic Beam; Canonical dual finite element method; Semi-definite programming.

Nonconvex variational problems have always presented serious challenges not only in numerical analysis, but also in computational mechanics and engineering sciences. By numerical discretization techniques, nonconvex variational problems are linked with certain nonconvex global optimization minimization problems. Due to the lack of global optimality condition, conventional numerical methods and direct approaches cant solve these problems deterministically. The popular primal-dual interior point methods suffer from uncertain error bounds in nonconvex analysis because of the intrinsic duality gaps produced by traditional duality theories. Therefore, most nonconvex minimization problems are considered as NP-hard in global optimization and computer sciences. Unfortunately, this fundamental difficulty is not fully recognized in computational mathematics and mechanics due to the significant gap between these fields.

Canonical duality theory is a newly developed, potentially powerful methodological theory which can transfer general multi-scale nonconvex problems in R n to a unified convex dual problem in continuous space R m with m = n and without duality gap. The associated triality theory provides extremality criteria for both global and local optimal solutions, which can be used to develop powerful algorithms for solving general nonconvex variational problems. This talk will present a canonical dual finite element method (CD-FEM) for solving general nonconvex variational problems. The speaker will show that by using Gao-Strangs complementary-dual principle and mixed finite element discretization, the general nonconvex variational problem can be reformulated as a min-max optimization problem of a saddle function. Based on the triality theory and the semi-definite programming method, a canonical primal-dual algorithm is proposed. Detailed application will be illustrated by post buckling problem of a large elastic deformations of beam, which is governed by a fourth order nonlinear differential equation. The total potential energy of this beam is a double-welled nonconvex functional with two local minimizers, representing the two buckled states, and one local maximizer representing the unbuckled state. Numerical results show that our algorithm can produce very stable solutions for both global minimizer and local maximizer. However, the local minimizer is very sensitive to numerical discretization and the external loads. The triality theory has been verified by using mixed finite element interpolations.

The theory, method and results presented by this talk should bring a some fundamentally new insights into nonconvex analysis, global optimization, and computational mathematics

Numerical solution of multiparameter spectral problems by high order finite different schemes

Pierluigi Amodio, Giuseppina Settanni

Dipartimento di Matematica, Università di Bari, Italy
pierluigi.amodio@uniba.it, giuseppina.settanni@uniba.it

Keywords. ordinary differential equations, boundary value problems, multiparameter spectral problems, finite differences.

We report on the progress achieved in the numerical simulation of self-adjoint multiparameter spectral problems for ordinary differential equations. We describe a method to define a discrete problem by means of High Order Finite Difference Schemes and discuss its numerical solution. Based on this approach, we also define an iterative method to compute approximations of the parameters by means of the solution of a set of problems converging to the original one.

Different test problems are considered to emphasize the behavior of the proposed algorithm. The obtained results are compared with those known in literature.

Acknowledgements.

This research was supported by the project ?Equazioni di Evoluzione: analisi qualitativa e metodi numerici? of the Dipartimento di Matematica, Università di Bari.

References

[1] P. Amodio, T. Levitina, G. Settanni, E. Weinmüller, Numerical simulation of the whispering gallery modes in prolate spheroids. *Computer Physics Communications* **185** (2014), pp. 1200–1206.

[2] P. Amodio, G. Settanni, Variable-step finite difference schemes for the solution of Sturm-Liouville problems. *Communications in Nonlinear Science and Numerical Simulation* **20** (2015), pp. 641–649.

[3] P. Amodio, G. Settanni, A matrix method for the solution of Sturm-Liouville problems. *Journal of Numerical Analysis, Industrial and Applied Mathematics*, **6** (2011), pp. 1–13.

[4] B. Plestenjaka, C.I. Gheorghiub, M.E. Hochstenbach, Spectral collocation for multiparameter eigenvalue problems arising from separable boundary value problems. *Journal of Computational Physics*, **298** 2015, pp. 585–601

Optimizing Sensor Cover Energy for Directional Sensors

Annabella Astorino, Manlio Gaudioso, Giovanna Miglionico

ICAR-CNR, Rende, Italy
DIMES-Universitá della Calabria, Rende, Italy
DIMES-Universitá della Calabria, Rende, Italy
astorino@icar.cnr.it, gaudioso@dimes.unical.it,
gmiglionico@dimes.unical.it

Keywords. Directional sensors; Lagrangian relaxation; Lagrangian heuristics; MINLP.

We present a mixed integer non linear programming formulation of the Directional Sensors Continuous Coverage Problem (DSCCP), where a given set of targets in a plane are to be covered by a set of sensors whose location is known in advance. Sensors are supposed to be directional, that is characterized by a discrete set of possible radii and aperture angles. Decisions to be made are about orientation (which in our approach can vary continuously), radius and aperture angle of each sensor, taking into account possibility of keeping one or more sensors switched off. The objective is to get minimum cost coverage of all targets. We incorporate into the objective function penalty cost for possibly uncovered targets.

We prove NP-hardness of DSCCP and introduce a Lagrangian relaxation model. We design a dual ascent procedure based on acting on one multiplier at a time accompanied by a heuristics to find a feasible solution at each ascent iteration. Finally we report the results of the implementation of the method on a set of test problems.

Optimization by Populations of Collaborative Local Searchers

Roberto Battiti, Mauro Brunato

DISI, University of Trento, Italy
Lobachevsky State University of Nizhny Novgorod, Russia
{battiti,brunato}@disi.unitn.it

Keywords. Local search optimization, Global optimization, Algorithm portfolio.

We propose a heuristic global optimization technique (Collaborative Reactive Search Oprimization, CoRSO) which combines combinatorial and continuous local search. The combinatorial component, based on Reactive Search Optimization, generates a trajectory of binary strings describing search districts. Each district is evaluated by random sampling and by selective runs of continuous local search. A reactive prohibition mechanisms guarantees that the search is not stuck at locally optimal districts.

The continuous stochastic local search is based on the *Inertial Shaker* method: candidate points are generated in an adaptive search box and a moving average of the steps filters out evaluation noise and high-frequency oscillations.

The overall subdivision of the input space in a tree of non-overlapping search districts is adaptive, with a finer subdivision in the more interesting input zones, potentially leading to lower local minima.

Finally, a portfolio of independent *CoRSO* search streams (*P-CoRSO*) is proposed to increase the robustness of the algorithm.

An extensive experimental comparison with Genetic Algorithms and Particle Swarm demonstrates that *CoRSO* and *P-CoRSO* reach results which are fully competitive and in some cases significantly more robust.

NOTE: an extended version of this work has been submitted to Informatica journal and is currently under review.

Acknowledgements.

The research in this paper was supported by the Russian Science Foundation, project no. 15–11–30022 "Global optimization, supercomputing computations, and applications."

GENOPT 2016: Design of a GENeralization-based Challenge in Global OPTimization

Roberto Battiti, Yaroslav Sergeyev, Mauro Brunato, Dmitri Kvasov

DIMES, University of Calabria, Italy
DISI, University of Trento, Italy
Lobachevsky State University of Nizhny Novgorod, Russia
{battiti,brunato}@disi.unitn.it, {yaro,kvadim}@dimes.unical.it

Keywords. Optimization contest, Benchmarks, Generalization.

While comparing results on benchmark functions is a widely used practice to demonstrate the competitiveness of global optimization algorithms, fixed benchmarks can lead to a negative *data mining* process. The motivated researcher can "persecute" the algorithm choices and parameters until the final designed algorithm "confesses" positive results for the specific benchmark.

To avoid this negative effect, the GENOPT contest benchmarks are based on randomized function generators, designed for scientific experiments, with fixed statistical characteristics but individual variation of the generated instances. The generators are available to participants for off-line tests and online tuning schemes, but the final competition is based on random seeds communicated in the last phase through a cooperative process. A scientific presentation and discussion of the methods and results will be part of a dedicated workshop at the LION 10 conference. The GENOPT challenge has the following goals:

Scientific learning and dynamic scoring The challenge is a joint, continued learning effort. Non-experts are encouraged to enter, see preliminary results, learn from their peers.

Open results Results are publicly visible, the better techniques are presented in scientific publications, benchmark functions remain available for future experimentation.

Diversity of approach A dangerous habit of some communities is to encourage only internal comparisons: GA against GA, PSO versus PSO... On the contrary, the larger the diversity of approach, the faster the scientific progress.

Seamless participation Effort in participating in the challenge is minimized, so that a researcher can concentrate on producing novel research.

We present the detailed design of the challenge as well as the most notable results obtained by participants.

Acknowledgements.

The research in this paper was supported by the Russian Science Foundation, project no. 15–11–30022 "Global optimization, supercomputing computations, and applications."

Min-Max Optimization for determining Optimal Parameters in Magnetic Spacecraft Stabilization via Attitude feedback

Renato Bruni[a], Fabio Celani[b], Stefano Lucidi[a]

a. Dep. of Computer Control and Management Engineering Antonio Ruberti, Sapienza University of Rome, Roma, Italy.
b. School of Aerospace Engineering, Sapienza University of Rome, Roma
bruni@dis.uniroma1.it, fabio.celani@uniroma1.it, lucidi@dis.uniroma1.it

Keywords. Derivativefree Optimization; Min-Max Problems; Spacecraft Attitude Control.

Spacecraft attitude control is a crucial task in astronautics. It is obtained by means of different types of actuation mechanisms. In particular, magnetic actuators are widely used for the generation of attitude control torques. They consist of current-driven coils rigidly placed on the spacecraft, which operate due to the interaction between the magnetic moment generated by the coils and the Earth's magnetic field. The attitude is stabilized by using a feedback control. Some control parameters must be determined. Usually, parameters are found with a trial-and-error approach within the huge search space of all their possible values. However, this approach requires a very inconvenient search, and nonetheless only a small portion of the search space is actually explored.

We propose here an innovative systematic approach for finding the control parameters: we aim at minimizing the settling time of the attitude error. Since settling time depends also on initial conditions, the optimal parameters for specific initial conditions may be not optimal for different conditions. Therefore, we search for a robust solution by minimizing the settling time obtained under the worst initial conditions by solving a min-max problem.

This problem is quite difficult, since the solution of the main minimization problem needs the solution of a maximization problem at every evaluation of its objective function. There are also two additional difficulties: settling time is discontinuous, and moreover it cannot be expressed in analytical form as function of control parameters and initial conditions.

We propose a derivative-free method for tackling this min-max problem. We use two derivative free algorithms for solving the main problem and the calculation of the objective. These algorithms use no first order information of the problem functions and try to take into account the particular structure of the min-max problem. Computational results obtained in a case study are very promising.

Region-of-interest tomography: a nonsmooth regularization approach based on shearlets

Tatiana A. Bubba†, Federica Porta‡, Gaetano Zanghirati‡, Silvia Bonettini‡

†Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università di Modena e Reggio Emilia
‡Dipartimento di Matematica e Informatica, Università di Ferrara
†,‡ INdAM-GNCS – Gruppo Nazionale per il Calcolo Scientifico
tatiana.bubba@unimore.it, federica.porta@unife.it, gaetano.zanghirati@unife.it, silvia.bonettini@unife.it

Keywords. Region-of-interest tomography; Nonsmooth optimization; Proximal-gradient algorithms.

In computed tomography (CT) applications, the possibility to reduce the X-ray dosage, while shortening the scanning time, is particularly relevant for biomedical imaging, where X-ray exposure comes with health hazards for patients. Region-of-interest (ROI) tomography has the potential to reduce the X-ray dosage, by considering only those rays meeting a region-of-interest, namely by truncating projection measurements. This makes the ROI reconstruction problem rather challenging, due to the severe ill-posedness and the presence of noise which compromise the stability of traditional CT reconstruction algorithms [1]. In order to obtain stable reconstructions, we introduce two convex optimization models which differ for the differentiability or the nondifferentiability of the objective function and are both based on *shearlets* regularizers [2].

For the solution of these convex problems, we analyze the very recently proposed *variable metric inexact line-search algorithm* (VMILA) [3]. VMILA is a proximal-gradient method, which enables the inexact computation of the proximal point defining the descent direction.
By using simulated data from fan-beam CT geometry and real data, we evaluate the goodness of both the models in terms of the quality of the reconstructions provided. In particular we investigate which technique is more effective in recovering the desired features of the image and in avoiding unwanted artifacts. Finally we prove that the considered approaches are insensitive to the location of the ROI and remain stable also when the ROI size is rather small.

References

[1] Clackdoyle R., Defrise M. (2010) *Tomographic Reconstruction in the 21st century. Region-of-interest reconstruction from incomplete data.* IEEE Signal Processing, 60:60–80.
[2] G. Kutyniok G., Labate D. (2012) *Shearlets. Multiscale Analysis for Multivariate Data.* Birkhäuser, Boston, MA (USA).
[3] Bonettini S., Loris I., Porta F., Prato M. (2016) *Variable metric inexact line-search based methods for nonsmooth optimization.* SIAM Journal on Optimization, in press.

Quasi-Newton Multipoint and Interpolation Methods with Line Search for Solving Nonlinear Equations

Oleg Burdakov, Ahmad Kamandi

Linköping University, Linköping, Sweden
Razi University, Kermanshah, Iran
oleg.burdakov@liu.se, ahmadkamandi@gmail.com

Keywords. Systems of nonlinear equations; quasi-Newton methods; line search.

We consider multipoint [1, 2] and interpolation [3] methods for solving systems of nonlinear equations. They approximate the Jacobian matrix using quasi-Newton updates. Due to their ability to more completely utilize the information gathered at the previous iterations about the Jacobian matrix, these methods are especially efficient in the case of expensive functions. Their local convergence is known to be superlinear. We apply a line search strategy proposed in [4] to make them globally convergent and justify this theoretically. Results of numerical experiments are presented. They show that the considered methods are more efficient than Broyden's method globalized in the same way.

References

[1] Gay D.M., Schnabel R.B. (1977) Solving systems of nonlinear equations by Broyden's method with projected updates. In *Nonlinear Programming 3* (ed by Mangasarian O.L. et al.), Academic Press, New York, pp. 245–281.

[2] Burdakov O.P. (1986) On superlinear convergence of some stable variants of the secant method. *ZAMM — Journal of Applied Mathematics and Mechanics*, Vol. 66, pp. 615–622.

[3] Burdakov O.P. (1997) A greedy algorithm for the optimal basis problem. *BIT Numerical Mathematics*, Vol. 37, pp. 591–599.

[4] Li D-H., Fukushima M. (2000) A derivative-free line search and global convergence of Broyden-like method for nonlinear equations. *Optimization Methods and Software*, Vol. 13, pp. 181–201.

Solving aircraft conflicts by continuous optimization and mixed-integer nonlinear programming

Sonia Cafieri[1,2], Andrew Conn[3], Marcel Mongeau[1,2]

[1] ENAC, MAIAA, F-31055 Toulouse, France, [2] Université de Toulouse, IMT, F-31400 Toulouse, France, [3]IBM Watson Research Center, NY
sonia.cafieri@enac.fr, arconn@us.ibm.com, marcel.mongeau@enac.fr

Keywords. Penalty function approach; Mixed-Integer Nonlinear Programming; Aircraft conflict avoidance.

Aircraft conflict detection and resolution in en-route flights, where an aircraft conflict is a loss of separation between aircraft trajectories, is crucial to ensure flight safety and remains a challenging problem in Air Traffic Management (ATM). Taking into account the increasing air traffic on the world scale and its impact on air traffic controllers' workload, a higher level of automation in ATM urgently needs to be introduced to deal with aircraft conflict avoidance. This problem still deserves investigation from both the identification of suitable mathematical models and the development of efficient solution methods [1, 2].

In the present work, we propose two novel optimization formulations, where the decision levers are both aircraft speed changes and heading angle changes. The first one is based on Mixed-Integer Nonlinear Programming (MINLP). MINLP appears particularly suitable in the considered context, as it enables to consider simultaneously continuous variables (aircraft speeds, heading angles, etc.) as well as integer ones (in particular, binary, to model logical choices), and to model complex nonlinear constraints characterizing ATM systems (pairwise aircraft separation). The second formulation we propose is a purely continuous optimization one, where we introduce a penalty function, tailored to the problem at hand, to deal with the aircraft separation constraints.

Numerical results on a set of problem instances validate the proposed approaches while highlighting the versatility of the proposed models.

Acknowledgements. This research was supported by grant ANR 12-JS02-009-01 "ATOMIC" by French National Research Agency.

References

[1] S. Cafieri and N. Durand. Aircraft deconfliction with speed regulation: new models from mixed-integer optimization. *Journal of Global Optimization*, 58(4):613–629, 2014.

[2] L. Pallottino, E. Feron, and A. Bicchi. Conflict resolution problems for air traffic management systems solved with mixed integer programming. *IEEE Transactions on Intelligent Transportation Systems*, 3(1):3–11, 2002.

Emergence of linguistic-like structures in one-dimensional Cellular Automata

Fabio Caldarola, Francesca Bertacchini, Eleonora Bilotta,
Pietro Pantano, Leonardo Renteria Bustamante

University of Calabria, ponte P. Bucci, 87036 Arcavacata di Rende (CS), Italy
caldarola@mat.unical.it, francesca.bertacchini@unical.it,
eleonora.bilotta@unical.it, pietro.pantano@unical.it,
lfrenteriax@hotmail.com

Keywords. Cellular Automata; Glider; Regular Domain; Complex Rules; Linguistic Structures.

We present an analytical model of Cellular Automata (CA) that uses the metaphor of natural language to explore the organizational complexity of CA systems. Starting with the basic elements, the CA states, we analyze how such data form strings of different complexity in the parameter space of all the possible couplings of these basic elements. Linguistic structures emerge that have precise rules of coupling and different levels of complexity. The metaphor of the language allows each CA to generate new strings continually, which are linguistically acceptable within the system. The reduction of a CA into a natural language allows an extreme economy and creativity: since once the basic elements and their combination rules are obrained it is possible to have an almost limitless range of patterns.
This work highlights a new approach to the construction of CA languages with criteria very similar to those found in biological systems or natural languages. In particular it is based on emerging behaviors and production rules set out by the same system, rather than formally made by a computational one (like in Turing machine or Chomsky's hierarchy). These rules of composition within a CA show the presence of an emerging language, which is proposed as a higher-level description than the simple rule of evolution and is typical of biological and natural self-organizing systems.

References

[1] Bilotta E., Lafusa E., Pantano P. (2010) Searching for complex CA rules with Gas. *Complexity*, Vol. 8(3), pp. 56–67.
[2] Bilotta E., Pantano P. (2010) *Cellular Automata and Complex Systems: Methods for Modelling Biological Phenomena*. Hershley, New York.
[3] Wolfram S. (1984) Universality and Complexity in Cellular Automata. *Physica D*, Vol. 10, pp. 1–35.

Preconditioning strategies for Nonlinear Conjugate Gradient methods, based on Quasi-Newton updates

Andrea Caliciotti, Giovanni Fasano, Massimo Roma

Dipartimento di Ingegneria Informatica, Automatica e Gestionale, SAPIENZA - Università di Roma, via Ariosto 25 – 00185 Roma, Italy
Department of Management, University Ca' Foscari of Venice, S. Giobbe, Cannaregio 873 – 30121 Venice, Italy
Dipartimento di Ingegneria Informatica, Automatica e Gestionale, SAPIENZA - Università di Roma, via Ariosto 25 – 00185 Roma, Italy
caliciotti@dis.uniroma1.it, fasano@unive.it, roma@dis.uniroma1.it

Keywords. Approximate Inverse Preconditioners; Preconditioned Nonlinear Conjugate Gradient; Large Scale nonconvex optimization; Quasi–Newton updates.

In this work we address new preconditioning strategies for Nonlinear Conjugate Gradient (NCG) methods, for large scale unconstrained optimization. We propose a family of preconditioners with a twofold purpose: on one hand, drawing inspiration from the class of Approximate Inverse preconditioners, we collect information from the NCG iterations, in order to generate an approximate inverse Hessian. On the other hand, we also try to convey information from quasi-Newton updates. In particular, for general large scale nonconvex functions, since storage is limited, we are only allowed to use information from a reduced number of previous iterations. This implies that a careful use of the latter information is sought. In particular, at any iteration of the NCG we consider preconditioners based on new low-rank quasi-Newton symmetric updating formulae, obtained as by-product of the NCG iterations. We also try to investigate the role of each component of our preconditioners, which contributes to define our proposal. An extensive numerical experience is performed on a large selection of CUTEst test set.

References

[1] Andrei N. (2007) Scaled memoryless BFGS preconditioned conjugate gradient algorithm for unconstrained optimization. *Optimization Methods and Software*, Vol. 22, pp. 561–571.
[2] Buckley B., Lenir A. (1983) QN-like variable storage conjugate gradients. *Mathematical Programming*, Vol. 27, pp. 155–175.
[3] Fasano G., Roma M. (2013) Preconditioning Newton-Krylov methods in nonconvex large scale optimization. *Computational Optimization and Applications*, Vol. 56, pp. 253–290.

A CA model for beach morphodynamics

C. R. Calidonna[1], M. De Pino[1], S. Di Gregorio[2,1], F. Gullace[1], D. Gulli[1], V. Lupiano[3]

[1]Inst. Clim. and Atm. Science–CNR, Ind. Area 15, 88046 Lamezia T. (CZ)
[2]DiMaCS;[3]DiBEST University of Calabria, 87036 Arcavacata (CS); Italy
(cr.calidonna,m.depino,d.gulli)@isac.cnr.it,
cicciogullace@yahoo.it, (dig,lupianov)@unical.it

Keywords. Cellular Automata; Coastal dynamics, simulation.

CAs coastal dynamics is a very complex system, computer simulation is a valid approach to plan real action. During SIGIEC Project a new Macroscopic Cellular Automata was designed i.e. RUSICA[1] for morphodynamics studies of the beaches. MCA [2] methodology, used for investigating natural macroscopic systems, is an alternative approach to PDE. Through local interactions of their constituent parts MCA operating on different specification levels to be compared to experimental data. Simulation allowed to study the dynamics and modified orography with artificial solutions for erosion contrast as at Porto Cesareo (Apulia Italy). $RUSICA =< R, X, S, P, \gamma >$ in this successive version [1] is a three dimensions MCA, where R defines the space portion, tessellated in regular hexagonal cells, where dynamical system evolves. X is the cell neighbouring conditions, specified by its adjacent cells. S is the set of cell states, that describe the features of the corresponding portion of space in terms of substates, the third dimension is implicit in some substates. Relevant cell substates are altitude, water depth, sand layer thickness, average kinetic energy of sea water, sea water average sand concentration, suspended sand flows. P is the set of global parameters, they include the temporal MCA clock, the cell apothem, the energy reflection and transmission coefficients, parameters of sand mobilization and deposit. The transition function γ computes sand erosion, transport and deposition. Interesting simulation results modeling atmospheric processes, wave energy and bathymetry allow to capture main results qualitatively compared to real occurred erosional events.

Acknowledgements.
PON 2007-2013 SIGIEC PON01 02651.

References

[1] Calidonna et al. (2015) RUSICA Initial Implementations: Simulation Results of Sandy Shore Evolution in Porto Cesareo, Italy, AIP Conference Proc., in press.
[2] Di Gregorio, Serra (1999) An empirical method for modelling and simulating some complex macroscopic phenomena by Cellular Automata. *Fut. Gen. Comp. Syst.*, Vol. 16, pp. 259-271

Domain Decomposition Methods for a Class of Integro-Partial Differential Equations

Giovanna Califano, Dajana Conte

University of Salerno, via Giovanni Paolo II,132 Italy
University of Salerno, via Giovanni Paolo II,132 Italy
gcalifano@unisa.it, dajconte@unisa.it

Keywords. Fractional diffusion-wave equations; Schwarz methods; Domain decomposition.

Schwarz Waveform Relaxation (WR) methods have been mainly developed and analysed for several kinds of PDEs [1, 2, 3], and consist in decomposing the spatial domain into subdomains(Domain Decomposition technique) and solve iteratively time dependent problems on subdomains, exchanging information at the boundary. Domain Decomposition methodology is well suited for parallelization on architectures such as GPUs or multicore CPUs.We first analyse the convergence behaviour of the classical Schwarz Waveform Relaxation method applied to fractional diffusion-wave equations,showing that Dirichlet boundary conditions at the artificial interfaces inhibit the information exchange between the subdomains and therefore slow down the convergence of the method. So, we construct optimal Schwarz WR methods, by providing the transmission conditions which assure convergence in a finite number of iterations.

Acknowledgements.
This research was supported by GNCS-INdAM.

References

[1] Gander M.J., Zhao H. (2002) Overlapping Schwarz waveform relaxation for the heat equation in n dimensions. *BIT*, Vol. 42, pp. 779-795.

[2] Gander M.J., Halpern L. and Nataf F. (2003) Optimal Schwarz waveform relaxation for the one dimensional wave equation. *SIAM J.Numer.Anal.*, Vol. 41, pp. 1643–1681.

[3] Gander M.J., Rohde C. (2005) Overlapping Schwarz waveform relaxation for convection-dominated nonlinear conservation laws. *SIAM J.Sci.Comput.*, Vol. 27, pp. 415–439.

Interlacing and monotonicity of zeros of orthogonal polynomials briefly revisited

K. Castillo, F. R. Rafaeli

CMUC, Department of Mathematics, University of Coimbra, 3001-501 Coimbra, Portugal
Departamento de Matemática, Universidade Federal de Uberlândia, 38408–100 Uberlândia, Minas Gerais, Brazil
kenier@mat.uc.pt, rafaeli@ufu.br

Keywords. Orthogonal polynomials; Monotonicity of zeros; Strum's comparison theorem; Markov's theorem.

In the nineteenth century, *orthogonal polynomials on the real line* (OPRL) have attracted deep interest especially since they exhibit rather comprehensive and very attractive analytic properties, such as e.g. their distribution of zeros. The zeros of the classical OPRL (those associated with the names of Jacobi, Laguerre, and Hermite) have been studied since 1886 when Markov and Stieltjes published their thorough pioneering works on this subject. However, for instance, Markov's theorem on monotonicity of zeros does not consider the cases with parameters in the singular part of the measure. In this sense, a natural open problem was pointed out in 1989 by the 2015 AMS Fellow, M. E. H. Ismail: Extend Markov's theorem to the case when the measure is given by

$$\omega(x,\tau)dx + d\nu(x,\tau),$$

where $\nu(\cdot,\tau)$ is a jump function or step function. The first answer to this problem was given recently by the authors. In this didactical talk we discuss this and other results on interlacing and monotonicity of zeros, in the context of OPRL, paying special attention to the flexibility and versatility of Markov's theorem on monotonicity of zeros of OPRL and Sturm's comparison theorem on zeros of Sturm-Liouville functions.

References

[1] Castillo K., Rafaeli F. R. (2015) On the discrete extension on Markov's theorem on monotonicity of zeros. *Electron. Trans. Numer. Anal.*, Vol. 44, pp. 271–280.
[2] Lun Y. C, Rafaeli F. R. (2014) Inequalities for zeros of Jacobi polynomials via Sturm's theorem: Gautschi's conjectures. *Numer. Algor*, Vol. 67, pp. 549–563.
[3] Szegő G. (1975) *Orthogonal Polynomials*. 4th edn. Amer. Math. Soc. Coll. Publ., Providence.

On the Fourth-Order Accurate Approximations of the Solution of the Dirichlet Problem for Laplace's Equation in a Rectangular Parallelepiped

Emine Celiker, Adiguzel A. Dosiyev

Middle East Technical University, Northern Cyprus Campus, 99378 Kalkanli, Güzelyurt, TRNC, Mersin 10, Turkey
Near East University, Near East Boulevard, Nicosia, TRNC, Mersin 10, Turkey
eceliker@metu.edu.tr, adiguzel.dosiyev@emu.edu.tr

Keywords. 3D Laplace equation; cubic grids on parallelepiped; 15−point scheme; interpolation for harmonic functions; discrete Fourier transform

An interpolation operator is proposed for the approximate solution of the Dirichlet problem for Laplace's equation in a rectangular paralellepiped. For the solution of the boundary value problem on the nodes required for the construction of the operator, a 15−point scheme is applied on the cubic grid.

The construction of the operator is based on homogeneous orthogonal-harmonic polynomials in three variables. It is proved that when the boundary functions on the faces of the rectangular parallelepiped are from the Hölder classes $C^{4,\lambda}$, $\lambda \in (0,1)$, and their second and fourth derivatives obey additional compatibility conditions implied by Laplace's equation on the edges, the solution obtained by the constructed operator has fourth-order accuracy with respect to mesh size. The proposed interpolation operator can also be applied as a matching operator in overlapping versions of domain decomposition, composite grids and combined methods.

The difference problem's solution on the nodes used for the interpolation operator is calculated by the fourth-order accurate formula derived on the basis of the discrete Fourier transform.

Nonlinear Reduced-Order Modeling with Contractivity and Monotonicity Properties

Saifon Chaturantabut*, Gun Srijuntongsiri**

*Department of Mathematics and Statistics, Faculty of Science and Technology, Thammasat University, Thailand
**School of Information, Computer, and Communication Technology (ICT) Sirindhorn International Institute of Technology (SIIT), Thammasat University, Thailand
saifon@mathstat.sci.tu.ac.th , gun@siit.tu.ac.th

Keywords. Differential equations; Model reduction; Proper orthogonal decomposition; Discrete empirical interpolation; Contractivity; Monotonicity.

Model reduction approaches have been recently proposed to substantially decrease the computational complexity of many large-scale dynamical systems, particularly arising from partial differential equations. However, most existing efficient approaches for nonlinear systems may not directly preserve the important properties of the original systems. This work derives a nonlinear reduced-order modeling that preserves the contractivity and monotonicity properties. These properties will be shown to guarantee the existence and uniqueness of the reduced-order solution, as well as provide some certain conditions that preserve the stability of the original system. The derivation of the proposed methodology is based on modifying an interpolatory projection approach, called discrete empirical interpolation method, and enforcing a symmetric structure of the system through a minimization problem. The efficiency and accuracy of the proposed method are illustrated through the numerical tests of two nonlinear models that describe the catalytic reaction and the process of phase separation problems.

Acknowledgements.
This research was supported by The Thailand Research Fund (TRF) grant for new researcher: Grant No. TRG5880216.

Properties of the Numerical Algorithms for Problems of Quantum Information Technologies: Benefits of Deep Analysis.

Chernyavskiy Andrey[2,1], Khamitov Kamil[1], Teplov Alexey[1], Voevodin Vadim[1], Voevodin Vladimir[1]

[1]Lomonosov Moscow State University, Moscow, Russia
[2]Institute of Physics and Technology, Russian Academy of Sciences, Moscow, Russia
andrey.chernyavskiy@gmail.com

Keywords. Algorithms, parallel computing, quantum information.

In recent years, quantum information technologies (QIT) showed great development. Different areas of QIT like quantum computers and cryptography lead to the fascinating applications inaccessible to classical approaches. Although, the way of the implementation faces the serious difficulties, some of which are challenging computational tasks. We analyze algorithmic properties of such tasks.

One of the main peculiarities is the exponential growth of necessary classical resources, and this is the reason to use modern supercomputers. In addition, the origins of quantum nature not only lead to the well-known quantum parallelism, but also to the highly parallel structure of classical computations in QIT. However, it is not so simple to use it efficiently, and the main goal of the work is fighting against this problem by using the deep and broad analysis of the algorithms.

We consider the modeling of one- and two-qubit transforms of the many-qubit quantum state as an example of algorithms. These transformations compose the basis of quantum computations and, consequently, are the most critical kernels of many important QIT applications.

The analysis of the algorithms consists of two parts: theoretical and experimental. Theoretical part includes features like sequential and parallel complexity, macro structure, and visual informational graph. Experimental part was made by using the petascale Lomonosov supercomputer (Moscow State University, Russia) and includes the analysis of locality and memory access, scalability and the set of more specific dynamic characteristics of realization.

It is important to note, that we use the methodology of the open encyclopedia of parallel algorithmic features Algowiki (algowiki-project.org) for the analysis of algorithms. This approach allows us to obtain bottlenecks and generate ideas of serious efficiency improvement.

Acknowledgements.

This project is carried out with the financial support of the Russian Science Foundation, Agreement No 14-11-00190.

Numerical Simulation of Unidirectional Models of Lasers

Raimondas Čiegis, Shalva Amiranashvili, Mindaugas Radziunas

Vilnius Gediminas technical university, Vilnius, Lithuania
WIAS, Berlin, Germany
rc@vgtu.lt, shalva@wias-berlin.de

Keywords. Finite difference method; forward Maxwell equations; numerical analysis.

We present and analyze different numerical algorithms for solution of the forward Maxwell equations (FME)

$$(\partial_z + \widehat{\beta} V^{-1} \partial_\tau) F + \frac{4n_2}{3c} \partial_t (F^3) = 0. \tag{1}$$

describing a propagation of laser wave packets. A special emphasis is given for applications to nonlinear fiber-optics. Here $E(z,t) = F(z,\tau)$ defines a polarized wave, $\tau = t - z/V$ is so-called retarded time.

Our main goal is to select appropriate numerical solvers for solution of this problem and to compare the efficiency of different strategies when they are used to solve the FME and the generalized nonlinear Schrödinger equations [1]. We investigate the optimality of the following alternatives: a) the finite difference methods versus pseudo-spectral methods; b) full approximation algorithms versus splitting algorithms; c) parallel MPI and OpenMP implementations [2].

The main numerical challenge deals with construction of robust and accurate numerical solvers for nonlinear terms of (1), which are describing a nonlinear interaction in FME. Special upwind type monotone and TVD approximations are applied and tested. Results of computational experiments are presented and a dynamics of complicated laser wave interactions is simulated. We note that some nonlinear effects can be resolved only by using the new FME model.

Acknowledgements.

This research was supported by the grant (No. MIP-074/2015) from the Research Council of Lithuania.

References

[1] Amiranashvili Sh., R. Čiegis, M. Radziunas (2015) Numerical methods for a class of generalized nonlinear Schrödinger equations. *Kinetic and Related Models*, Vol. 8, pp. 215–234.

[2] Radziunas M., R. Čiegis. (2014) Effective numerical algorithm for simulations of beam stabilization in broad area semiconductor lasers and amplifiers. *Math. Model. Anal.*, Vol. 19, pp. 627–646.

Lexicographic Multiobjective Linear Programming using Integer Grossone Powers

[1]Marco Cococcioni, [1]Massimo Pappalardo, [2,3]Yaroslav D. Sergeyev

[1]University of Pisa, Pisa, Italy
[2]University of Calabria, Rende (CS), Italy
[3]Lobachevsky State University of Nizhni Novgorod, Russia
m.cococcioni@iet.unipi.it, m.pappalardo@di.unipi.it, yaro@dimes.unical.it

Keywords. Lexicographic Multiobjective Optimization; Linear Programming; Simplex method; *Grossone*.

In Lexicographic Multi-Objective Linear Programming (LMOLP) problems multiple linear objective functions are provided along with their associated priorities. Traditional LMOLP problems are solved by solving a sequence of single objective LP problems. This approach is time consuming. On the other hand, it is well-known that the set of objectives can be transformed into a single objective, by using a weighted sum of the single objectives, where lower weights are associated to less important objectives [1]. The advantage of using this approach is that, once the problem is reduced to a single-objective LP, standard algorithms (like simplex methods/internal point methods) can be run *only once*. However, determining such weights is challenging and, no general methods exist to choose them up to now. In this work we show how the use of *grossone* [2] allows one to create a single objective function, which is, in this case, a linear combination of non-positive powers of *grossone*, without the need to specify *any finite weight*. The first (most important) objective is weighted by 1, the second by $grossone^{-1}$, the third by $grossone^{-2}$, etc. After this transformation, the single-objective LP problem can be solved *only once*. This problem is solved by using the simplex method, extended to the case of *grossone* numbers [2], implemented in Matlab. Thus we have obtained the advantage of having to solve only one LP problem, without the need to provide any finite weight to the algorithm. A theoretical analysis of the proposed methodology has been also performed.

Acknowledgements. The research of Ya.D. Sergeyev was supported by the Russian Science Foundation, project No 15-11-30022 "Global optimization, supercomputing computations, and applications".

References

[1] Sherali H.D. (1982) Equivalent weights for lexicographic multiobjective programs: characterization and computations. *Eur J Oper Res*, Vol. 11, pp. 367-379

[2] Sergeyev Ya.D. (2009) Numerical computations and Mathematical modelling with infinite and infinitesimal numbers, *J of Applied Mathematics and Computing*, Vol. 29, pp. 177-195.

Characterization of one-dimensional cellular automata rules through topological network features

Lou D'Alotto, Clara Pizzuti

Department of Mathematics and Computer Science, York College, City University of New York, Jamaica, NY 11451, USA
National Research Council of Italy, Institute for High performance Computing and Networking, Via P. Bucci 7-11C, 87036 Rende (CS), Italy
ldalotto@bc.cuny.edu, pizzuti@icar.cnr.it

Keywords. one-dimensional cellular automata; Wolfram classification; Gilman classification.

Cellular automata are discrete computational systems having enormous potentials in modeling complex systems. Since their introduction by von Neuman they have attracted researchers from different fields and extensively studied. Wolfram, especially, investigated the dynamic behavior of one-dimensional automata and defined four types of behavior: homogeneous (Class I), periodic (Class II), chaotic (Class III) and complex (Class IV). This classification characterizes rules of each class by using parameters obtained by computer simulations. A different classification of linear automata into three classes $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$, has been proposed by Gilman. It is based on a measure theoretic classification approach that assigns a rule to a class by considering the probability of choosing a configuration that will stay close to a fixed initial configuration after the evolution of that rule for a time period. The relationship between Wolfram and Gilman classifications is not clear. Gilman asserts that Classes I and II lie in $\mathcal{A} \cup \mathcal{B}$, Class IV cannot be in $\mathcal{A}$ or $\mathcal{C}$, thus it must be in $\mathcal{B}$ and that Class III could be in $\mathcal{C}$. In this paper we investigate the relation between Wolfram and Gilman classes by exploiting the network representation of one-dimensional cellular automata. Each elementary rule is modeled with a network obtained by evolving the rule for a number of steps by starting from a random initial configuration. Some topological features of the graph generated after the evolution are computed and used to characterize the rules. Classification models by using machine learning classification methods are built and trained on the four Wolfram's classes already known. Then classification of Gilmans' rules in one of the four classes of Wolfram are obtained by applying the models to each rule.

References

[1] Wolfram W. (1994) *Cellular automata and complexity.* Addison-Wesley.
[2] Gilman R. H. (1987) Classes of Linear Automata. *Ergodic Theory and Dynamical Systems*, Vol. 7, pp. 105–118.

The Use Fast Legendre Transform Algorithm for Numerical Simulation of Nonlinear Waves and Structures

Igor Demin, Sergey Gurbatov

Lobachevsky State University of Nizhny Novgorod, Gagarin Ave., 23, Nizhny Novgorod, 603950, Russian Federation
demin@rf.unn.ru, gurb@rf.unn.ru

Keywords. Fast Legendre Transform; nonlinear waves; Burgers equation.

The theory of nonlinear waves and structures is a very extensive and constant developing field of physics (especially radiophysics and mathematical physics). It has many specific applications. Among them there are both the well-known problems of acoustics, electrodynamics and plasma physics, and the less-known problems, such as surface-growth description, dynamics of turbulence and development of a gravitational instability of the large-scale distribution of matter in the Universe. A wide range of phenomena arising here have led to the development of a variety of mathematical methods, which are effective in addressing various kinds of nonlinear fields and waves [1].

In the simplest model of propagation of finite amplitude sound waves are described by the well-known Burgers equation. In studies of nonlinear wave propagation an important problem is to find the waveform of the asymptotic wave at long time after the preparation of the initial wave or at long distance from the source emitting the wave. The main difficulty in numerical analysis of stochastic nonlinear acoustic waves is the large cost of computer time and a large amount of memory for all numerical models describing the shock wave. One of optimization algorithms for computing is the use of the Fast Legendre Transform, which will significantly reduce the number of required operations in comparison with standard methods.

The goal of the present paper is the numerical investigation of the evolution of anisotropic regular and random structures and waves in the multi-dimensional Burgers equation.

Acknowledgements.

This research was supported by the Russian Science Foundation (Grant 14-12-00882).

References

[1] Gurbatov S.N., Rudenko O.V., Saichev A.I. (2011) *Waves and Structures in Nonlinear Nondispersive Media: General Theory and Applications to Nonlinear Acoustics.*Springer Verlag, Berlin.

A method of harmonic extension for computing the generalized stress intensity factors for Motz's problem

Adiguzel A. Dosiyev

Near East University, Near East Boulevard, Nicosia, TRNC, Mersin 10, Turkey
adiguzel.dosiyev@emu.edu.tr

Keywords. Motz's problem; Laplace equation; singularity problem; Block method; stress intensity factor; error analysis

For more than half a century, many researches have been testing on Motz's problem as a benchmark of singularity problems for verifying the efficiency of different approaches. The solution of Motz's problem has a singularity at the origin due to the change of boundary conditions, and it can be expanded as

$$u(r,\theta)=\sum_{j=0}^{\infty}a_j r^{j+\frac{1}{2}}\cos\left(\left(j+\frac{1}{2}\right)\theta\right), \tag{1}$$

where r and θ are polar coordinates centred at the singular point. The unknown constants a_j are often called generalized stress intensity factors (GSIFs) in the theory of elasticity. A highly accurate approximation of these coefficients are very important because they are valuable in different applied problems such as fracture mechanics, and also to get a highly accurate approximation of the solution and its derivatives.

In this talk, the solution of the problem on a special polygon is harmonically extended to the sector with center at the singular vertex. This is followed by an integral representation of the extended harmonic function in this sector, through the Poisson kernel, which is approximated by the mid-point quadrature rule. Using the extension formulae,we obtain a system of linear equations for the solution values on the quadrature nodes. It is proved that the solution of this system converges to the exact value exponentially with respect to the number of quadrature nodes. By using approximate values on the nodes, we present an explicit formula for the GSIFs which also converges exponentially. For the numerical justification of the obtained theoretical results Motz's problem is used, and comparisons are made with the best existing results in the literature. Moreover, the extremely accurate series segment solution is obtained by taking an appropriate number of calculated GSIFs.

A Comparison of SuperLU Solvers on the Intel MIC Architecture

Mehmet Tuncel[a,b], Ahmet Duran[a], M. Serdar Celebi[b], Bora Akaydin[b], Figen Ö. Topkaya[c]

a. Istanbul Technical University, Department of Mathematics, Istanbul 34469, Turkey
b. Istanbul Technical University, Informatics Institute, Istanbul 34469, Turkey
c. Bilgi University, Department of Industrial Engineering, Istanbul 34469, Turkey
tuncelm@itu.edu.tr, aduran@itu.edu.tr, mscelebi@itu.edu.tr

Keywords. Direct solver; large sparse matrix; numerical linear algebra.

In many science and engineering applications, problems may result in solving a sparse linear system $AX = B$. For example, SuperLU_MCDT, a linear solver, was used for the large penta-diagonal matrices for 2D problems and hepta-diagonal matrices for 3D problems, coming from the incompressible blood flow simulation ([1]). It is important to test the status and potential improvements of state-of-the-art solvers on new technologies. In this work, sequential, multithreaded and distributed versions of SuperLU solvers ([2]) are examined on the Intel Xeon Phi coprocessors using offload programming model at the EURORA cluster of CINECA in Italy and they work well. We consider a portfolio of test matrices containing patterned matrices from UFMM ([3]) and randomly located matrices ([4]). This architecture can benefit from high parallelism and large vectors. We find that the sequential SuperLU benefited up to 45 % performance improvement from the offload programming depending on the sparse matrix type and the size of transferred and processed data.

Acknowledgements.
This research was supported by the PRACE-1IP project funded in part by the EUs 7th Framework Programme (FP7/2007-2013) under grant agreement no. RI-261557 and the Project 2010PA1756 awarded under the 18th Call for PRACE Preparatory Access.

References

[1] Duran A., Celebi M.S., Piskin S., and Tuncel M. (2015) Scalability of OpenFOAM for bio-medical flow simulations, *J. of Supercomputing*, Vol. 71(3), pp. 938–951.
[2] Li X. S., Demmel J. W., Gilbert J. R., Grigori L., Shao M., and Yamazaki I., (1999) SuperLU Users' Guide, Tech. Report UCB, Computer Science Division, University of California, Berkeley, CA, update: 2011.
[3] Davis T.A., The University of Florida sparse matrix collection.
[4] Duran A., Celebi M.S., Akaydin B., Tuncel M. and Oztoprak F. (2013) Analysis of SuperLU solvers on the Intel MIC architecture, PRACE PN: RI-261557, PRACE-1IP Extension white paper, Evaluations on Intel MIC, WP 135.

Parallel Numerical Parameter Optimization Algorithm for a Dynamical System

Ahmet Duran[a], Mehmet Tuncel[a,b]

a. Istanbul Technical University, Department of Mathematics, Istanbul 34469, Turkey
b. Istanbul Technical University, Informatics Institute, Istanbul 34469, Turkey
aduran@itu.edu.tr, tuncelm@itu.edu.tr

Keywords. Continuous optimization; parallel algorithm; economic model.

We propose a new hybrid algorithm for parameter estimation and implement it using Message Passing Interface (MPI) parallel programming. In particular, we introduce a scalable parallel nonlinear parameter optimization algorithm with parameter pools for a nonlinear dynamical system. For example, we apply the algorithm to the asset flow differential equations (AFDEs) that have been developed and analyzed since 1989 (see [1], [2], [3], and references contained therein). We generate time series pairs as proxy to market price and net asset value by using random walk simulation where the volatilities of the time series are similar to that of real closed-end funds traded on New York Stock Exchange (NYSE). When we apply the algorithm by using simulations for a set of time series, we observe that the computed optimal parameter values, average number of quasi-Newton iterations, the average nonlinear least squares errors, and the average maximum improvement factors can converge certain values within corresponding small ranges, after oscillations. Moreover, we tested for 64, 128, 256 and 512 cores using the 512 initial parameter vectors. We achieved speed-up for the time series to run up to 512 cores.

Acknowledgements.
This research was supported by the PRACE-2IP project funded in part by the EUs 7th Framework Programme (FP7/2011-2014) under grant agreement no. RI-283493 (see [4]) and the Project 2010PA2507 awarded under the 19th Call for PRACE Preparatory Access. The computing resources of ITU UHeM were also used.

References

[1] Caginalp G. and Ermentrout B. (1991) Numerical studies of differential equations related to theoretical financial markets, *Appl. Math. Lett.*, Vol. 4, pp. 35–38.
[2] Caginalp G. and Balenovich D. (1999) Asset flow and momentum: deterministic and stochastic equations, *Phil. Trans. R. Soc.* Vol. 357, pp. 2119–2133.
[3] Duran A. and Caginalp G. (2008) Parameter optimization for differential equations in asset price forecasting, *Optim. Methods Softw.*, Vol. 23, pp. 551–574.
[4] Duran A. and Tuncel M. (2014) Scalable parallel nonlinear parameter optimization algorithm with parameter pools, PRACE PN: RI-283493, PRACE-2IP Extension white paper, Scalable Algorithms, WP 185.

Optimization in Modeling the Ribs-Bounded Contour from Computer Tomography Scan

Gintautas Dzemyda, Mykolas J. Bilinskas

Institute of Mathematics and Informatics, Vilnius University, Akademijos str. 4, LT-08663 Vilnius, Lithuania
gintautas.dzemyda@mii.vu.lt, mykolas.bilinskas@mii.vu.lt

Keywords. Optimization; computer tomography; modeling; curve fitting.

In medicine, many decisions on diagnostics and evaluation of effectiveness of the treatment are made via analysis of images. Image data comes from medical techniques such as radiology, echoscopy, magnetic resonance, thermovision, tomography, etc.

Computed tomography (CT) is a technology allowing the inside of objects to be spatially viewed using computer-processed X-rays. It is very important in medical diagnostics because it shows human internal organs without cutting, e.g. brain, liver, prostate. CT scans are 3D images a collection of 2D images (slices), representing slices by transversal plane. When evaluating the effectiveness of the treatment, pre- and post- treatment CT scans must be made (for the same patient) and compared by aligning (registering) these two (or more) scans [1]. We consider the slices where ribs are visible, because many important internal organs are located here: liver, heart, stomach, pancreas, lung, etc. [2].

We present a method for analyzing CT scan slices: a mathematical model that describes the ribs-bounded contour was created and the problem of approximation is solved by finding out the optimal parameters of the model using least-squares. Such model allows us registration of images independently on the patient position on the bed and on the radio-contrast agent injection.

The model of ribs-bounded contour of particular slice of CT scan has nine parameters whose values can be varied seeking to find the best approximation of the contour. Various optimization approaches are discussed. The experiments indicate that the objective function is multiextremal.

References

[1] Graf F., Kriegel H.-P., Schubert M., Plsterl S., Cavallaro A. (2011) 2D image registration in CT images using radial image descriptors. In Proceedings of the *14th International Conference on Medical Image Computing and Computer-Assisted Intervention, MICCAI 2011* (ed. by Fichtinger G. et al.), Toronto (Canada), p. 607–614.

[2] Bilinskas M.J., Dzemyda G., Trakymas M. (2015) Computed tomography image analysis: the model of ribs-bounded contour. In Proceedings of the *International Conferences in Central Europe on Computer Graphics, Visualization and Computer Vision, WSCG 2015* (ed. by Skala V.), Plzen (Czech Republic), p. 81–84.

Polarity for Quadratic Hypersurfaces and the Conjugate Gradient method: relation with degenerate and non-degenerate cases

Giovanni Fasano

Department of Management, University Ca' Foscari of Venice, S. Giobbe, Cannaregio 873 – 30121 Venice, Italy
fasano@unive.it

Keywords. Polarity in homogeneous coordinates; Quadratic hypersurfaces; Conjugate Gradient method; Singular linear systems.

In this work we consider some results from Projective Geometry, in order to propose a geometric standpoint for a class of iterative methods widely adopted within convex unconstrained optimization. In particular, we focus on the Theory of Polarity for quadratics, and recast some of its geometric results in view of the properties of the Conjugate Gradient method. This method is an efficient Krylov-based iterative procedure, for the solution of positive definite linear systems. We first show that by means of the Theory of Polarity several results for conjugate directions can be easily proved and extended also in the indefinite case. Moreover, we investigate the latter issue also in case the system matrix is singular, which corresponds to a degenerate case within the Theory of Polarity. We remark that in case the system matrix is singular, the use of Polarity needs some care, inasmuch as Polarity no more defines a one-to-one correspondence between points and hyperplanes of the projective space. We want to investigate if the latter anomaly might be fruitfully exploited in optimization frameworks, with possibly a couple of final purposes. First, we want to prove the existence of conjugate directions, along with their properties, also in the degenerate case. Then, we want to provide some hints in order to develop iterative efficient methods for singular systems.

References

[1] G. Fasano (2015) A framework of conjugate direction methods for symmetric linear systems in optimization. *Journal of Optimization Theory and Applications*, Vol. 164, pp. 883–914.

[2] Hestenes, Stiefel E. (1952) Methods of conjugate gradients for solving linear systems. *Journal of Research of the National Bureau of Standards*, Vol. 49, pp. 409–435.

Approximate Computation of the Green's Function of Transverse Vibration of the Composite Rods

Serife Faydaoglu, Valery G. Yakhno

Department of Mathematics, Buca Faculty of Education, Dokuz Eylul University, Buca, 35150 Izmir, Turkey
Electrical and Electronics Engineering Department, Faculty of Engineering, Dokuz Eylul University, Buca, 35160 Izmir, Turkey
serife.faydaoglu@deu.edu.tr, valery.yakhno@deu.edu.tr

Keywords. Fourth order boundary value problem; Green function; Eigenvalue; Eigenfunction.

Let us consider the equation of the transverse vibration of a composite rod:

$$\rho(x)A(x)\frac{\partial^2 u}{\partial t^2} + \frac{\partial^2}{\partial x^2}(E(x)I(x)\frac{\partial^2 u}{\partial x^2}) = \delta(x - x_0, t), \tag{1}$$

where $x \in (0, l)$ is the space variable, $t \in R$ is the time variable; $\delta(x-x_0, t)$ is the Dirac delta function, concentrated at $x = x_0$, $t = 0$; $x_0 \in (0, l)$ is the parameter; $\rho(x)$ is the mass density, $A(x)$ is the cross-sectional area, $E(x)$ is the modulus of elasticity, $I(x)$ is the moment of inertia of the cross-section, $u(x, t; x_0)$ is the function of the transverse motion. We assume that $\rho(x), E(x), A(x), I(x)$ are piecewise constant functions having jumps at a given point $x = r$. The main problem of the paper is to find a generalized function $u(x, t; x_0)$ satisfying equation (1), the initial data $u|_{t<0} = 0$, the boundary conditions $u|_{x=0} = \frac{\partial u}{\partial x}|_{x=0} = 0$, $u|_{x=l} = \frac{\partial u}{\partial x}|_{x=l} = 0$ and the interface conditions $u|_{x=r-0} = u|_{x=r+0}$, $\frac{\partial u}{\partial x}|_{x=r-0} = \frac{\partial u}{\partial x}|_{x=r+0}$, $b_1\frac{\partial^2 u}{\partial x^2}|_{x=r-0} = b_2\frac{\partial^2 u}{\partial x^2}|_{x=r+0}$, $b_1\frac{\partial^3 u}{\partial x^3}|_{x=r-0} = b_2\frac{\partial^3 u}{\partial x^3}|_{x=r+0}$. Where b_1, b_2 are constants. The method of approximate computation of this problem is suggested in the paper. This method consists of the derivation the finite number of eigenvalues and corresponding to then eigenfunctions of a spectral problem and then finding an approximate solution of (1) in the boundary and interface conditions in the form of the Fourier series with a finite number of terms. The results of the paper continue the research of the work [1, 2].

References

[1] Faydaoglu S., Yakhno V.G. (2012) Applications of finite and infinite Fourier series in heat processes with impulse data, Applied Mathematics and Computation Vol. 218, pp. 8120-8130.

[2] Faydaoglu S., Guseinov G.Sh. (2003) Eigenfunction Expansion for a Sturm- Liouville Boundary Value Problem with Impulse, International Journal of Pure and Applied Mathematics, Vol. 8, pp. 137-170.

Finite-time parameters estimation of the Chua system

Giuseppe Fedele[1], Francesco Chiaravalloti[2], Luigi D'Alfonso, Gaetano D'Aquila[3], Gilberto Pin[4], Thomas Parisini[5]

[1]DIMES, [2]DIMEG, University of Calabria, Italy
[3]GiPStech s.r.l, Italy, [4]Electrolux Professional S.p.A, Italy
[5] Dept. of Electrical and Electronic Engineering, Imperial College London, UK
(giuseppe.fedele,francesco.chiaravalloti)@unical.it,
(l.dalfonso,g.daquila)@gipstech.com, gilbertopin@alice.it,
t.parisini@gmail.com

Keywords. Chua's circuit; Volterra kernels; adaptive control.

Chaotic systems have attracted the attention of the recent research due to their potential applications in secure communication, laser system, electronic chemistry, neurophysiology and ecology [1]. The reconstruction problem consists in recovering the underlying variables and the unknown parameters from a partial knowledge of a chaotic system [2], i.e. it is desired to extract some physical parameters and to estimate some non available states from the available system outputs. In this work, the unknown set of parameters of the Chua system is recovered under the hypothesys that the voltages of the capacitors are available. To this end, focusing on the differential equations, the Volterra kernel-based approach is used to perform an estimation without the uncertainty of the unmeasurable derivatives. The kernel-based method designs a class of Bivariate Causal Non-asymptotic Kernel (BC-NK) to form the Volterra integral operator, providing a finite-time parameter estimation for continuous-time linear systems, annihilating the effects of the unknown initial conditions. Inspired by the idea of [3], in this paper, the Volterra operator with BF-NK is used to achieve a joint parametric estimation of the Chua system parameters with arbitrary non-asymptotic convergence.

References

[1] Fedele G., Ferrise A., Chiaravalloti F. (2016) Uncertain master-slave synchronization with implicit minimum saturation level. *Applied Mathematical Modelling*, 40(2), pp. 1193–1198.

[2] Wu X., Wang Z. (2009) Estimating parameters of chaotic systems under noise-induced synchronization. *Chaos Solitons & Fractals*, 39, pp. 689–696.

[3] Pin G., Assalone A., Lovera M., Parisini T. (2016) Non-Asymptotic Kernel-Based Parametric Estimation of Continuous-Time Linear Systems. *IEEE Transactions on Automatic Control*, 61(2), pp. 360–373.

A heuristic approach to the maximum edge weight clique problem on sparse networks

Dalila B.M.M. Fontes, Sergiy Butenko, Mohammad Hosseinian

Texas A&M University, Department of Industrial and Systems Engineering, College Station, TX 77843-3131, United States
Faculdade de Economia, Universidade do Porto and LIAAD/INESC TEC, Porto, Portugal
dfontes@tamu.edu, butenko@tamu.edu, hosseinian@tamu.edu

Keywords. maximum edge weighted clique problem; combinatorial optimization; heuristic.

The maximum clique (MC) problem is to find the maximum sized subgraph of pairwise adjacent vertices in a given graph. MC is a prominent combinatorial optimization problem with many applications and has been shown to be NP-hard [2]. This work addresses a generalization of the MC, the maximum edge weighted clique (MEWC) problem, in which one wants to find a clique with maximum edge weight. The MEWC problem has long been discussed in the literature, but mostly addressing complete graphs. However, many applications exist in which many edges are missing, either due to some thresholding process or because they do not exist, for example in protein threading and alignment, market basket analysis, cells metabolic networks (see [1] and references therein). Not many studies have addressed the MEWC problem on sparse networks and most introduce dummy edges with large negative costs. We propose a 2-phase heuristic approach to efficiently find good solutions for the MEWC on sparse graphs, by taking advantage of the graph sparsity.

Acknowledgements.

This research was partially supported by project "NORTE-01-0145-FEDER-000020" - financed through North Portugal Regional Operational Programme (NORTE 2020), under the PORTUGAL 2020 Partnership Agreement, and the European Regional Development Fund (ERDF).

References

[1] Gouveia, L., Martins, P. (2015) Solving the maximum edge-weight clique problem in sparse graphs with compact formulations. *EURO Journal on Computational Optimization*, Vol. 3, pp. 1–30.

[2] Karp, R. M. (1972) *Reducibility among combinatorial problems*. Springer US.

Optimal Control of Constrained Nonholonomic Systems: adaptive time-grid refinement algorithms

Fernando ACC Fontes, LT Paiva

Universidade do Porto, Portugal
faf@fe.up.pt, ltpaiva@fe.up.pt

Keywords. Optimal control, Predictive control, Nonlinear systems, Real-time optimization, Adaptive algorithms, Time-mesh refinement.

We address optimal control problems for nonholonomic systems with state-constraints. These are challenging nonlinear problems for which the number of discretization points is a major factor determining the computational time. Also, the location of these points has a major impact in the accuracy of the solutions. We propose an algorithm that iteratively finds an adequate time-grid to satisfy some predefined error estimate on the obtained trajectories, which is guided by information on the adjoint multipliers.

The obtained results show a highly favourable comparison against the traditional equidistant-spaced time-grid methods, including the ones using discrete-time models. This way, continuous-time plant models can be used directly. The discretization procedure can be automated and there is no need to select a priori the adequate time step. Even if the optimization procedure is forced to stop in an early stage, as might be the case in real-time, we can still obtain a meaningful solution, although it might be a less accurate one.

Extension of the procedure to a Model Predictive Control (MPC) context is also discussed. By defining a time-dependent accuracy threshold, we can generate solutions that are more accurate in the initial parts of the receding horizon, which are the most relevant for MPC.

References

[1] Paiva, L.T., Fontes, F.A.C.C. (2015). Adaptive time-mesh refinement in optimal control problems with state constraints. *Discrete and Continuous Dynamical Systems*, Vol. 35(9), pp. 4553–4572.

Computational Fluid Dynamic Modelling of Horizontal Single Belt Casting (HSBC) of Steel Strips; Numerical and Modelling Issues.

Roderick I.L.GUTHRIE, Mihaiela ISAC

McGill Metals Processing Centre, McGill University, 3610 University Street, 2M040 Wong Bldg., Montreal, H3A0C5, Canada.
{Roderick.Guthrie,Mihaiela.Isac} @mcgill.ca

Keywords. Computational Fluid Dynamic; Numerical Modelling; Strip Casting.

Horizontal Single Belt Casting (HSBC) is a near net shape strip casting technology (1-20mm thick product) that is poised to gain significant prominence in the coming years, for both steel and aluminum sheet production. Fluid mechanics, and associated heat and mass transfer, are important aspects of any continuous casting process, and the HSBC process is no exception. In this study, 3D Computational Fluid Dynamics (CFD) simulations were developed, using ANSYS FLUENT 145, to predict various aspects of the HSBC process for low carbon liquid steels. Specific emphasis was placed on the effects of the substrates thermal and surface properties on strip quality, and solidification behavior. These numerical predictions were compared to experimental casting results on the HSBC simulator for low carbon steel strips.

It is predicted that the metal flow above the copper substrate (which is moving at 0.5 m/s), rapidly becomes iso-kinetic. Nevertheless, recirculating flows can be seen to form near the backwall meniscus, where the melt first contacts the moving belt. This recirculation is critical to keeping the melt fluid there, thereby preventing premature solidification and clogging in the nozzle region. The increase in effective viscosity to $10Pa.s$ ($10kg.m^{-1}s^{-1}$), generated by shearing flows, is significantly raised above steels molecular viscosity of $0.06Pa.s$. This contributed significantly to the stability of the meniscus at the back-gap, helping to prevent melt back-flow. Similarly, it aided in the development of iso-kinetic flows of steel with the moving substrate. Some of the uncertainties in this mathematical model will be highlighted, and suggestions are made regarding improvements needed in future mathematical modeling research.

Acknowledgements. This research was supported NSERC and companies supporting the McGill Metals Processing Centres research activities.

References

[1] S. Ge, M. Isac, R.I.L. Guthrie, The Computational Fluid Dynamic (CFD) Modeling of the Horizontal Single Belt Casting (HSBC) Processing of Al-Mg-Sc-Zr Alloy Strips, *Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science* (2015), October, Volume 46 B, pp 2264-2277.

[2] Roderick Guthrie, Mihaiela Isac, Horizontal Single Belt Casting of Aluminum and Steel, *Steel Research International, Special Issue: Science and Technology of Steelmaking.* Volume 85, Issue, pp 1291-1302, August 2014.

[3] R.I.L. Guthrie, M. Isac, D. Li, Roderick I. L. Guthrie, Mihaiela Isac, Donghui Li, "Ab-initio Predictions of Interfacial Heat Flows during the High Speed Casting of Liquid Metals in Near Net Shape Casting Operations", Proceedings of the Seetharaman Symposium, Sigtuna, June 15-17, 2010, Sweden, published in Steel Research International, October, Vol.81, 2010. pp 891-898.

Numerical Methods for Nonsmooth Boundary Value Problems in Contact Mechanics

Joachim Gwinner

Universität der Bundeswehr München, D-85577 Neubiberg, Germany
Joachim.Gwinner@unibw-muenchen.de

Keywords. Finite element method; nonconforming approximation; regularization methods.

In this talk we report on recent progress in the numerical treatment of various nonsmooth boundary value problems in continuum mechanics, including unilateral contact with Tresca friction and nonmonotone adhesion/delamination problems. The contribution is based on the recent paper [1] of the author and on recent joint work [2, 3] with N. Ovcharova.

Firstly in an appropriate vectorial Sobolev function space V, we deal with nonsmooth variational problems in the form: Find $\mathbf{u} \in \mathbf{K}$ such that for all $\mathbf{v} \in \mathbf{K}$,

$$a(\mathbf{u}, \mathbf{v}-\mathbf{u}) + \int_{\mathbf{\Gamma_c}} \mathbf{g}\,|(\gamma_{\mathbf{c}}\,\mathbf{v})_{\mathbf{t}}|\,\mathbf{ds} - \int_{\mathbf{\Gamma_c}} \mathbf{g}\,|(\gamma_{\mathbf{c}}\,\mathbf{u})_{\mathbf{t}}|\,\mathbf{ds} \geq \mathbf{l}(\mathbf{v}-\mathbf{u})\,,$$

where K is the convex closed subset of kinematically admissible displacements.

Secondly we are concerned with nonconvex nonsmooth variational problems in the form of a hemivariational inequality: Find $\mathbf{u} \in \mathbf{V}$ such that for all $\mathbf{v} \in \mathbf{V}$,

$$a(\mathbf{u}, \mathbf{v}-\mathbf{u}) + \int_{\mathbf{\Gamma_c}} \mathbf{f^0}(\mathbf{u}(\mathbf{s}), \mathbf{v}(\mathbf{s}) - \mathbf{u}(\mathbf{s}))\;\mathbf{ds} \geq \mathbf{l}(\mathbf{v}-\mathbf{u})\,.$$

Here f^0 stands for the Clarke generalized directional derivative of a locally Lipschitz function f.

References

[1] Gwinner J. (2013) *hp*-FEM convergence for unilateral contact problems with Tresca friction in plane linear elastostatics. *J. Comput. Appl. Math.*, Vol. 254, pp. 175–184.

[2] Gwinner J., Ovcharova N. (2015) From solvability and approximation of variational inequalities to solution of nondifferentiable optimization problems in contact mechanics. *Optimization*, Vol. 64, pp. 1683–1702.

[3] Ovcharova N., Gwinner J. (2014) A study of regularization techniques of nondifferentiable optimization in view of application to hemivariational inequalities. *J. Optim. Theory Appl.*, Vol. 162, pp. 754–778.

On the Complex HZ Method for the PGEP

Vjeran Hari, Josip Matejaš

University of Zagreb, Department of Mathematics, Bijenička cesta 30, 10000 Zagreb, Croatia
University of Zagreb, Faculty of Economics, Kennedyjer trg 6, 10000 Zagreb, Croatia
hari@math.hr, jmatejas@efzg.hr

Keywords. Generalized eigenvalue problem; HZ method; convergence.

We study the element-wise and the block Jacobi-type method for the positive definite generalized eigenvalue problem (PGEP) $Ax = \lambda Bx$, where A and B are complex Hermitian matrices and B is positive definite. Our research is devoted to derivation of the algorithms and to their global and asymptotic convergence analysis. The element-wise method is the proper complex generalization of the real HZ method, which is a variant of the Falk-Langemeyer (FL) method. The FL method is used for solving the definite GEP with real matrices. The HZ method further assumes that B has ones along the diagonal and it is designed to retain this property during iteration. When solving real PGEP, the FL method can be viewed as the fast-scaled version of the HZ method.

The real HZ method has proved to be very fast and stable when implemented as one-sided block Jacobi-type algorithm for solving the generalized singular value problem. Then it is highly parallelizable, so parallel shared memory versions of the algorithm are perfectly scalable, and their speedup almost solely depends on the number of cores used. It compares favorably to the LAPACK DTGSJA algorithm. That has been incentive for generalizing the method to cope with complex matrices.

The first results include the derivation of the element-wise complex algorithm and the proof of its asymptotic quadratic convergence. Our preliminary investigation shows that the global convergence of the method can be proved for a large class of generalized serial pivot strategies. We also intend to prove high relative accuracy of the method when both matrices are positive definite.

As for the block method, we intend to prove its global convergence for the same class of generalized serial strategies.

Acknowledgements.
This work has been fully supported by Croatian Science Foundation under the project IP-09-2014-3670.

Identifying Service Contexts for QoS Support in IoT-Service Oriented Software Defined Networks

Young Ju Heo, Won Sang Chin, Ju Wook Jang

Sogang University, Seoul, Korea
Sogang University, Seoul, Korea
Sogang University, Seoul, Korea
protoheo@sogang.ac.kr, mokey82@sogang.ac.kr, jjang@sogang.ac.kr

Keyword. Network; Application; Identification; IoT; SDN;.

An important challenge for supporting variety of applications in the Internet of Things is the network traffic engineering and virtual network technologies such as SDN(Software Defined Network)s. To assign virtual network, it require service context (QoS) however, identifying service context is not easy. For that reason, the proliferation of new applications use port numbers already known. (e.g HTTP = 80). In addition, the encrypted packets(e.g HTTPS) make it difficult to identify service contexts.

This paper presents an identifying scheme for service contexts from real network traffic to support service-oriented IoT network. We use statistical properties of newtrok traffic such as mean packet length, mean interpacket arrival time, and standard deviation interpacket arrival time to identify service contexts.(e.g. Video Streaming, Video Conference, File Transfer Service.) The contribution of our approach is in identifying services which have not been identified by previous methods.

We devise a scheme which incrementally add dimensions to separate services until all services are identified. For example, Video Streaming and FTP shows identical statistical properties when we examine by two dimensions(MPL: Mean Packet Length, MIAT: Mean Inter-Arrival Time), hence not separable. However, if we add one more dimension(SDIAT: Standard Deviation of Inter-Arrival Time), the two services can be clearly separated. Our scheme can be used to find out which traffic needs what QoS in combined traffics, which can be used for traffic engineering in SDN.

Acknowledgements.

This Work was supported by Institute for Information & communications Technology Promotion(IITP) grant funded by the Korea government(MSIP) (No. B0126-15-1051, A Study on Hyper Connected Self-Organizing Network Infrastructure Technologies for IoT Service).

References

[1] Maldeniya, S. L., Atukorale, A. S., & Vithanage, W. W. (2013, December). Network data classification using graph partition. In Networks (ICON), 2013 19th IEEE International Conference on (pp. 1-6). IEEE.

Teaching the arithmetic of infinity: a qualitative evaluation

Paola Iannone, Davide Rizza, Athina Thoma

Loughborough University, Mathematics Education Centre, UK
University of East Anglia, Dept of Philosophy, UK
University of East Anglia, School of Education, UK
P.Iannone@lboro.ac.uk, d.rizza@uea.ac.uk, A.Thoma@uea.ac.uk

Keywords. grossone; arithmetic of infinity; high school teaching.

We present the initial, qualitative results of the first school trial of the booklet *First steps in the Arithmetic of Infinity* (which presents, with exercises, some of the topics developed in [1, 2, 3, 4] and several paradoxes of infinity). This was carried out with a group of British Sixth Form students (age 16 to 18) and their Mathematics teachers. We consider the students' proficiency in handling arithmetical computations involving grossone, finding the sums of geometric series of a specified infinite length, and comparing two treatments of Thomson's lamp, with and without grossone respectively. We conclude by surveying the feedback received from teachers, which highlights the accessible and rewarding nature of the materials and suggests extensions thereof, to deal with core topics within the mathematics curriculum that involve a direct appeal to the concept of infinity (e.g. improper integrals).

References

[1] Sergeyev Ya.D. (2003) *The Arithmetic of Infinity.* Orizzonti Meridionali, Rende.
[2] Sergeyev Ya.D. (2008) 'A new applied approach for executing computations with infinite and infinitesimal quantities', *Informatica*, 19(4), 567-596.
[3] Sergeyev Ya.D. (2009) 'Numerical point of view on Calculus for functions assuming finite, infinite, and infinitesimal values over finite, infinite, and infinitesimal domains', *Nonlinear Analysis Series A: Theory, Methods & Applications*, 71(12), e1688-e1707.
[4] Sergeyev Ya.D. (2015) 'Un semplice modo per trattare le grandezze infinite ed infinitesime', *La Matematica nella Societ e nella Cultura: Rivista dellUnione Matematica Italiana*, Serie I, Vol.8, 111-147.

On the Iterative Processes in the Krylov-Sonneveld Subspaces

V.P.Il'in

The Institute of Computational Mathematics and Mathematical Geophysics, SBRAS,
Novosibirsk State University, Novosibirsk, Russia
ilin@sscc.ru

Keywords. Krylov-Sonneveld Subspaces; Iterative processes

The main objective of this paper is the algebraic analysis of the introduced dimensional reduction (IDR) algorithms for solving very large sparse non-symmetric SLAEs, which in recent decades have been investigated by many authors, as compared to the classical iterative preconditioned methods in the Krylov subspaces. The key idea of the IDR approach consists in constructing the so-called Sonneveld embedded subspaces of the decreasing dimensions, which is provided by periodical orthogonalization to a test fixed subspace. Sometimes such approaches are considered as alternative to the Krylov algorithms.

The main topics of the recent studies on modified Krylov methods include the orthogonalization techniques by means of using deflation subspaces, based on a low rank approximation of matrices. Such algorithms are efficiently applied to parallel domain decomposition methods, to solving discrete multi-dimensional boundary value problems, and called as aggregation, or coarse grid correction. We describe an application of these approaches for the multi-preconditioned semi-conjugate direction methods in the block Krylov subspaces and show that the considered class of iterative processes can be interpretated by the IDR conception, also, which means that the computed residuals are placed in the subspaces of the reduced dimensions.

EroCal 2.0: a dynamic distributed soil erosion model

Giulio Iovine[1], Alessio De Rango[2], Donato DAmbrosio[2], Oreste Terranova[1]
terranova@irpi.cnr.it

[1] CNR-IRPI of Cosenza (Italy)
[2] Department of Mathematics and Computer Science, University of Calabria, Rende (CS), Italy

Keywords. Modelling; Cellular Automata; Soil erosion

Soil erosion processes on the slopes may affect the socio-economic development of the territory. In the PON Research Project AlForLab, aimed at improving knowledge, inventorying, planning and managing of forestry resources in Calabria (Southern Italy), the simulation of rainfall-related processes has been dealt with through an innovative approach based on an integrated library that enables parallel computing. Within such a frame, a new model EroCal 2.0 has been implemented for simulating soil erosion process along the slopes. The model allows to handle processes at either slope or regional scale and it can operate either on single rainfall events (at sub-hourly scale) or on prolonged periods (at daily scale).

EroCal 2.0 is a Cellular Automata model that takes advantage of increasing accuracy of available data on environmental variables, and recent improvements of numerical tools. The model can simulate both rainfall events and related elementary processes along the slopes. It is physically-based and, in the present release, takes into account: spatial and temporal distribution of precipitation; interception by vegetation or other natural/manmade surfaces; evapotranspiration; storage in pools; surface runoff; infiltration; soil erosion. The mathematical description of the physical processes guarantees mass and energy balance.

The considered computational domains (atmosphere, slope surface, underground) are handled as dynamic, discretized systems according to a 3D-grid, in which dimensions are uniform in the plane and vertically variable. The evolution of the computational domains depends on the considered physical elementary processes, each one evolving according to a specific local rule. The global behaviour of the geo-hydrological phenomenon emerges from the combined simulation of the elementary processes.

The model is being tested on ideal and real case studies, selected from Calabrian forestry sectors. Its behaviour is also being compared with other models not CA-based - available in literature (e.g., EUROSEM, LISEM, GeoTop). Thanks to the adopted parallel computing environment, the time required for simulations allows for quasi-real time applications. Further developments are envisaged at modelling floods, mass-transport phenomena along slopes and channels, and related effects on slope stability.

Structure preserving finite difference scheme for the vortex filament motion

Tetsuya Ishiwata

Shibaura Institute of Technology, Fukasaku 307, Minuma-ku, Saitama , Japan
tisiwata@shibaura-it.ac.jp

Keywords. finite difference scheme; vortex filament; structure preserving method.

The Localized Induction models are simple models of vortex filament motion in three dimensional incompressible flow. They are approximated skeleton models obtained by the Biot-Savart law via a cut-off and a regularization in some sense and there is a hierarchy of Localized Induction approximation models. In this talk, we consider the first and the second models in the hierarchy, that is, Localized Induction Equation(LIE) [1] $x_t = x_s \times x_{ss}$ and the Moore-Saffman equation [2] $x_t = x_s \times x_{ss} + W[x_{sss} + \frac{3}{2}(x_{ss} \cdot x_{ss})x_s]$, and propose structure preserving finite difference schemes for these models. Here the space curve $x(s,t) = (x_1(s,t), x_2(s,t), x_3(s,t))$ (s: arc-length, t: time.) describes a position vector of the vortex filament in the fluid. These models have two important properties: one is the length-preserving property and the other is the energy structure. The first one means that the tangential vector of solution vector keeps its length. We show that the proposed scheme inherits the length-preserving and the energy structures from the original models. We also show some theoretical results on the scheme and numerical results.

Acknowledgements.

This research was supported by Grant-in-Aid for Challenging Exploratory Research (No. 24654026, 15K13461) and Grant-in-Aid for Scientific Research (B)(No. 15H03632).

References

[1] Arms R. J. and Hama F. R. (1965), Localized- Induction Concept on a Curved Vortex and Motion of an Elliptic Vortex Ring, *Phys. Fluids*, Vol. 8, pp. 553–559.

[2] Fukumoto Y. and Miyazaki T, Three-dimensional distortions of a vortex filament with axial velocity, *J. Fluid Mech.*, Vol. 222, pp. 269–416.

[3] Fuwa A., Ishiwata T. and Tsutsumi M. (2012), Finite difference scheme for the Landau-Lifshitz equation, *Japan J. Ind. Appl. Math.*, Vol. 29, pp. 83–110.

[4] Tani A. and Nishiyama T. (1997), Solvability of Equations for Motion of a Vortex Filament with or without Axial Flow, *Publ. RIMS, Kyoto Univ.*, Vol. 33, pp. 509–526.

Mining Feature-Opinion in Biased Online Community

Sunghyun Kang, Jiwan Seo, Seungjin Choi, Junho Kim, Sangyong Han

Department of computer science Engineering, Chungang Univ., Heukseok-dong, Dongjak-gu, Seoul, Korea
(asdf, jwseo, bethemoney, taki0112)@ec.cse.cau.ac.kr, hansy@cau.ac.kr

Keywords. decision making support system; inclination classification ; sentiment classification.

As the internet technology and social media are advancing rapidly, massive opinion is produced, shared and distributed through the online communities. This information is very important and valuable in making optimal decisions. However, these kind of communities get naturally and subtlety biased. This is quite normal and unavoidable as only a very limited number of active people are generating discussions and monopolizing the conversation while many other people are passive and just consume the information. This situation seems to be present in any online community with many members. As online community opinion is not a perfect representation of a real world due to inherent bias in it, it is very important to identify and remove bias effectively for an efficient and fair decision making system.

This paper takes a machine learning approach at identifying bias in these communities. The proposed system has two classifiers. The first one is the inclination classifier and the other one is the sentiment classifier. The machine learning based inclination classifier evaluate the polarity of each opinion and the sentiment classifier quantitatively identify the positiveness of the contents of each opinion. The proposed system is able to identify biased contents, and able to deliver a feature opinion which represent an un-biased real world view.

The proposed system is implemented in C and maintained in a digital curation system. Visualization system is also implemented using PhP, HTML and JavaScript. An expert analysis of two online communities were carried out and the results quantitatively show that the proposed system is able to mitigate biased opinion.

Acknowledgements.

This research was supported by the Chung-Ang University Research Scholarship Grants in 2015 and this research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Science, ICT and future Planning (NRF - 2015R1A2 A2A01005304)

The circumradius condition and its application

Kenta Kobayashi

Graduate School of Commerce and Manegement, Hitotsubashi University
Naka 2-1, Kunitachi, Tokyo 186-8601, Japan
kenta.k@r.hit-u.ac.jp

Keywords. Interpolation error constant; Finite element method; A priori error estimate.

Let $\mathcal{P}_1$ be the set of polynomials in two variables whose degree are at most 1. Let $T \in \mathbb{R}^2$ be any triangle with vertices p_i $i = 1, 2, 3$. Then, for a function $u \in W^{2,p}(T)$ $1 \leq p \leq \infty$ the $\mathcal{P}_1$ interpolation Πu on T is defined by $\Pi u(p_i) = u(p_i)$. Recentry, the following interpolation error estimate was given by [1, 2]:

$$\|u - \Pi u\|_{W^{1,p}(T)} \leq C_p R(T) |u|_{W^{2,p}(T)}$$

where $R(T)$ denotes the circumradius of T and C_p is a constant depends only on p.

The analysis of the interpolation error is particularly important for the error analysis of the finite element methods. This estimate shows that the finite element solution converges to an exact solution if the maximum circumradius of the triangular elements converges to zero. We call such situation "circumradius condition" and claimed that the circumradius condition is more essential than the well-known maximum angle condition for convergence of the finite element method. We extended these results to the higher order Lagrange interpolation [3].

In the presentation, we will introduce the circumradius condition and its application for the error estimation for the finite element method with Delaunay triangulation.

Acknowledgements.
This work was supported by JSPS Grant-in-Aid for Scientific Research (C) Grant Number 25400198.

References

[1] Kobayashi K., Tsuchiya, T. (2014) A Babuška-Aziz type proof of the circumradius condition. *Japan J. Indust. Appl. Math.*, Vol. 31, pp. 193–210.
[2] Kobayashi K., Tsuchiya, T. (2015) On the circumradius condition for piecewise linear triangular elements. *Japan J. Indust. Appl. Math.*, Vol 32, pp. 65–76.
[3] Kobayashi K., Tsuchiya, T. (2015) A priori error estimates for Lagrange interpolation on triangles. *Applications of Mathematics*, Vol. 60[5], pp. 485-499.

On a method of construction numerical integration formulas

Anatoliy G. Korotchenko, Valentina M. Smoryakova

N.I. Lobachevsky State University, Gagarin Av.23, 603950 Nizhni Novgorod, Russia
koangr@yandex.ru, smorykov@mail.ru

Keywords. Numerical integration formulas; optimal strategies.

The paper describes the problem of numerical integration formulas construction for stiff systems of differential equations. The domain of these equations can consist of intervals where the solution is substantially non-linear and intervals where the solution is close to constant. The calculation of the right part of stiff equations can be an expensive procedure. Therefore, it is necessary to minimize the number of calculations when creating numerical integration formulas. Moreover, the end of the integration procedure can be undefined a priori, but is defined during the integration process. Hence, the use of constant step integration is inexpedient.

The strategies of choosing integration step size are developed for the specific finite-difference schemes. They are designed so that the number of integration nodes is minimal on a fixed interval under the constraints defined by the precision of calculations. This minimization problem is formulated as a mathematical programming problem.

In a number of cases, it makes sense to use individual finite-difference formulas for some intervals instead of using the same one for the whole domain of stiff equations. Here each formula is optimal as mentioned above. Replacement of finite-difference formulas is performed while switching from one interval to another. Depending on the concrete finite-difference formula the estimate of the corresponding derivative is computed for each fixed interval. At the same time, it makes sense to use such switching within each interval maintaining optimal properties of the resulting formula. Various strategies of using the considered finite-difference formulas are derived from these facts.

The mentioned strategies are investigated and implemented for the defined set of finite-difference formulas. The computing experiment results are listed.

References

[1] Korotchenko A.G. (2011) On multistage mathematical programming problems. *Vestnik of Lobachevsky State University jf Nizhni Novgorod*, Vol. 1, pp. 183–187.

[2] Korotchenko A.G., Smoryakova V.M. (2013) Multistage mathematical programming problems. In Proceedings of the *International Conference "Numerical Computations: Theory and Algorithms"* (ed. by Dell'Accio F., Kvasov D.E., Sergeyev Ya.D.), Falerna (Italy), p. 88.

Numerical simulations of astrophysical problems on massively parallel supercomputers

Igor Chernykh, Igor Kulikov, Boris Glinskiy

Institute of Computational Mathematics and Mathematical Geophysics SB RAS,
Lvrentjeva ave. 6, Novosibirsk, Russia
chernykh@ssd.sscc.ru, kulikov@ssd.sscc.ru, gbm@sscc.ru

Keywords. high performance computing; computational astrophysics; massively parallel supercomputers.

Numerical modeling plays a key role in modern astrophysics. It is the main tool for the research of nonlinear processes and provides communication between the theory and observational data. Numerical simulation in astrophysics allows detailed investigation of the collision and evolution of galaxies. Modern supercomputers have given us the possibility of subgrid-scale astrophysics modeling that considers different physical effects such chemical kinetics, cooling/heating, and more. One of the most interesting developments in supercomputer technology at this moment is massively parallel supercomputers. The main concept of this technology is based on the possibility of massive usage of computation accelerators. In our work, we use a multicomponent hydrodynamic model of galaxies considering the chemodynamics of molecular hydrogen. For the description of a gas component we are using the single-speed multicomponent gravitational gas dynamics equations. The collisionless component is described by the first moments of the collisionless Boltzmann equation system. The Poisson equation is used for calculation of gravitational potential. The formation of molecular hydrogen is described by an ordinary differential equation. We are using the co-design technique for development of astrophysical code. As a result of this approach the efficiency of the parallel implemetation (weak scalability) is 75% for 53760 threads of 224 Intel Xeon Phi accelerators. Our tests show that only 9% of the total simulation time spent on MPI/OpenMP send/receive operations.

Acknowledgements.

This research was supported by Russian Foundation for Basic Research (grants 15-31-20150, 15-01-00508, 16-07-00434) and by Grant of the President of Russian Federation for the support of young scientists number MK 6648.2015.9.

References

[1] Kulikov, I.M., Chernykh, I.G., Snytnikov, A.V., Glinskiy, B.M., Tutukov, A.V. (2015) AstroPhi: A code for complex simulation of dynamics of astrophysical objects using hybrid supercomputers. *Computer Physics Communications*, Vol. 186, pp. 71–80.

An interval approach to compute Initial Value Problem

Le Mezo Thomas, Jaulin Luc, Zerr Benoit

ENSTA-Bretagne, LabSTICC, 2 rue Franois Verny, 29806 Brest, France
{thomas.le_mezo,luc.jaulin,benoit.zerr}ensta-bretagne.fr

Keywords. Guaranteed integration; initial-value problems; interval analysis; state equation.

We propose a new guaranteed interval approach for solving Initial Value Problem (IVP) for ordinary differential equations. The method is orthogonal to literature as we do not use the Picard operator nor any interval counterpart of integration method (Euler [2], Runge-Kutta [1] or Taylor [3]).

The method is based on a geometrical interpretation of the vector field infer from the IVP. By building a subpaving of the research space and by computing the value of the vector field inside each pave, we can iteratively compute a guaranteed solution of the IVP.

We will consider simple test-cases and will benchmark our new tool with other solvers.

Acknowledgments.

This research was supported by the French Government Defense procurement and technology agency (Direction Gnrale de l'Armement - DGA).

References

[1] A. Chapoutot and J. Alexandre dit Sandretto and O. Mullier (2015) *Dynibex, available at* , http://perso.ensta-paristech.fr/čhapoutot/dynibex/. ENSTA.

[2] R. E. Moore and H. Ratschek (1988) Inclusion function and global optimization II. *SIAM*.

[3] N. Revol and K. Makino and M. Berz (2005) Taylor models and floating-point arithmetic: proof that arithmetic operations are validated in COSY. Journal of Logic and Algebraic Programming. , Vol. 64, pp. 135–154.

A Cost Minimization Design of Non-conforming Control Charts

Supranee Lisawadi

Department of Mathematics and Statistics, Thammasat University, Pathumthani, 12120, Thailand
supranee@mathstat.sci.tu.ac.th

Keywords. Quality Control; Duncan Process; Shutdown Process; np-Charts; Loss-cost.

When it comes to statistics in the economic system that is relevant to the industry, statistics are taken into consideration in terms of quality inspection in the production process as well as satisfaction of consumers, which is available from quality control charting. These will be used as the criteria for determining the boundaries of the product quality control charts, which makes the lowest overall cost (Loss-cost) by creating functions under control charts and np-charts. It can be seen that values of various parameters in the control charts are necessary to consider from the boundaries. The scope of this analysis will give us the amount of random samples required to monitor the quality of the product. In addition, this study will be analyzed from two different situations: Duncan Process, which the processes will still operate during the search for the cause abnormalities, and Shutdown Process, which will be searched during the processes are shutdown. In conducting this study, we aim to determine the best condition and circumstances surrounding that result in the lowest loss-cost.

Equations Ordering Influence on Inexact and Quasi-Inverse Newton methods

Giulio Masetti[1,2], Silvano Chiaradonna[1] and Felicita di Giandomenico[1]

[1]Soft. Eng. and Depend. Comp. Lab., ISTI/CNR, Via G. Moruzzi 1, Pisa, Italy,
[2]Comp. Sci. Dep., University of Pisa, Largo B. Pontecorvo 3, Pisa, Italy.
Ref.: giulio.masetti@isti.cnr.it

Keywords. Jacobian-free Newton Method; Equation Ordering.

The Newton-Raphson method has a prominent role in applied science and engineering. For instance, it is involved in the solution of discretized systems of partial differential equations [1]. Given the system of non-linear equations $F(u) = 0$, if $F : \mathcal{R}^n \rightarrow \mathcal{R}^n$ is a continuously differentiable function, then one of the solutions can be found via the Newton-Raphson method. At each step of this iterative method, a linear system that involves the Jacobian J_F of F has to be solved. At increasing the size of the problem, solving with a direct method the linear system is often impractical (w.r.t. time or space complexity), even if the Jacobian is a sparse matrix. Therefore, in these cases iterative methods have been studied, where, differently from the classical method, the equation ordering becomes important. Studies are available on techniques employed in medium-size linear systems, such as the Gauss-Seidel method, where changes in equation ordering are exploited to gain in efficiency. Instead, Jacobian-free techniques for very large linear problems have not been investigated with respect to this aspect. One of the most effective in this category is the Inexact-Newton [2] that approximates the matrix-vector product $J_F(u)v$ with $[F(u + \sigma v) - F(u)]/\sigma$. Another is the Quasi-Inverse-Newton [3] that approximates the inverse of the Jacobian J_F^{-1} with a diagonal matrix and solves directly the linear system. We prove that the equation ordering affects these last two methods and we present a preliminary analysis of how the equation ordering impacts on the two variants for a simple case study. Interestingly, the equations ordering does not only affect the efficiency in reaching a solution, but also the solution itself. We believe this is an important result, that the users of these methods need to be aware of.

References

[1] Brown, Peter N. and Saad, Youcef (1990) Hybrid Krylov methods for nonlinear systems of equations. *SIAM J. Sci. Statist. Comput.*, Vol. 11, pp.450–481.

[2] Knoll, Dana A. and David E. Keyes (2004) Jacobian-free NewtonKrylov methods: a survey of approaches and applications, *J. Comput. Physics*, Vol. 193, Num. 2, pp 357–397.

[3] Waziri, M. Y. and Leong, W. J. and Hassan, M. A. and Monsi, M. (2010) *J. Numer. Math. Stoch.*, Vol 2, Num. 1, pp 54–63.

Numerical methods for solving initial value problems on the Infinity Computer

F. Mazzia, Ya.D. Sergeyev, F. Iavernaro, P. Amodio, M.S. Mukhametzhanov

Dipartimento di Matematica, Università degli studi di Bari, Italy,
DIMES, Università della Calabria, Italy
francesca.mazzia@uniba.it,yaro@si.dimes.unical.it,
felice.iavernaro@uniba.it,pierluigi.amodio@uniba.it,marat@dimes.unical.it

Keywords. Ordinary Differential Equations, Initial Value Problems, numerical infinitesimals, Infinity Computer.

New algorithms for the numerical solution of Ordinary Differential Equations (ODEs) with initial conditions are proposed. They are designed for work on a new kind of a supercomputer – the Infinity Computer, – that is able to deal numerically with finite, infinite and infinitesimal numbers. Due to this fact, the Infinity Computer allows one to calculate the exact derivatives of functions using infinitesimal values of the stepsize. As a consequence, the new methods described are able to work with the exact values of the derivatives, instead of their approximations. Within this context, a variant of a one-step multi-point method closely related to the classical Taylor formulae is considered. It is shown that the new formula is order three accurate, though requiring only the first two derivatives of $y(t)$. To get numerical evidence of the theoretical results, test problems are solved by means of the new methods and the obtained results are compared with the performance of Taylor methods of order up to four.

Acknowledgements. Work supported by the Russian Science Foundation, project No.15-11-30022 "Global optimization, supercomputing computations, and applications" and the Università degli studi di Bari "Aldo Moro", project "Equazioni di Evoluzione: analisi qualitativa e metodi numerici".

References

[1] Ya.D. Sergeyev, M.S. Mukhametzhanov, F. Mazzia, F. Iavernaro, and P. Amodio. (2016). Numerical methods for solving initial value problems on the Infinity Computer. *International Journal of Unconventional Computing*, in press.

[2] P. Amodio, F. Iavernaro, F. Mazzia, M.S. Mukhametzhanov, and Ya.D. Sergeyev. (2016). A generalized Taylor method of order three for the solution of initial value problems in standard and infinity floating-point arithmetic. Mathematics and Computer in Simulation, in press.

[3] Ya.D. Sergeyev. (2011). Higher order numerical differentiation on the infinity computer. *Optimization Letters*, 5(4):575–585.

[4] Ya.D. Sergeyev. (2013). Solving ordinary differential equations by working with infinitesimals numerically on the infinity computer. *Applied Mathematics and Computation*, 219(22):10668–10681.

Cyber-Physical Approach to the Network-Centric Robotics Control Task

Vladimir Muliukha, Alexander Ilyashenko, Vladimir Zaborovsky, Alexey Lukashin

Russian State Scientific Center for Robotics and Technical Cybernetics, Tikhoretsky 21, St.Petersburg, Russia
Peter the Great St.Petersburg Polytechnic University, Polytechnicheskaya 29, St.Petersburg, Russia
vladimir@mail.neva.ru, ilyashenko.alex@gmail.com, vlad@neva.ru, lukash@neva.ru

Keywords. cyber-physics; robot; network-centric approach; cloud computing; actor.

Complex engineering tasks concerning control for groups of mobile robots are developed poorly. In our work for their formalization we use cyber-physical approach, which extends the range of engineering and physical methods for a design of complex technical objects by researching the informational aspects of communication and interaction between objects and with an external environment [1]. The paper analyzes network-centric methods for control of cyber-physical objects. Robots or cyber-physical objects interact with each other by transmitting information via computer networks using preemptive queueing system and randomized push-out mechanism [2],[3]. The main field of application for the results of our work is space robotics. The selection of cyber-physical systems as a special class of designed objects is due to the necessity of integrating various components responsible for computing, communications and control processes. Network-centric solutions allow using universal means for the organization of information exchange to integrate different technologies for the control system.

Acknowledgements.
This research was supported by the RFBR grant 15-29-07131 ofi-m.

References

[1] Zaborovsky V., Lukashin A., and Muliukha V. (2015) A chapter. In *Cyber-Physical Systems From Theory to Practice* (ed. by Danda B. Rawat, Joel J. P. C. Rodrigues, and Ivan Stojmenovic), CRC Press, USA, pp. 259–282

[2] Muliukha V., Ilyashenko A., Zayats O., and Zaborovsky V. (2015) Preemptive Queuing System with Randomized Push-Out Mechanism. *Communications in Nonlinear Science and Numerical Simulation*, Vol. 21, Issues 1–3, pp. 147–158.

[3] Ilyashenko A., Zayats O., Muliukha V., and Laboshin L. (2014) Further investigations of the priority queuing system with preemptive priority and randomized push-out mechanism. *Lecture Notes in Computer Science* Vol. 8638, pp. 433–443.

Spontaneous pattern formation in broad-area lasers

Anton Krents , Dmitry Anchikov, Nonna Molevich, Anton Pakhomov

Samara State Aerospace University, Moskovskoe shosse 34, Samara, Russia
Lebedev Physical Institute, Novo-Sadovaya 221, Samara, Russia
krenz86@mail.ru

Keywords. Pattern formation; broad-area lasers; optical vortex.

The paper studies the spontaneous formation of nonlinear optical patterns in broad area lasers. Spatiotemporal transverse dynamics of the laser is described by the Maxwell-Bloch (MB) equations. The instability of the steady-state solution leads to pattern formation. Two different types of instabilities were observed analytically (Hopf and Wave). 2D numerical simulation of the MB equations with the random initial conditions has been performed using a split-step Fourier method and periodic boundary conditions. The MB equations consist of the linear and nonlinear operators. Linear and nonlinear operators act independently at very small time. Linear part includes 2D Laplace operator and can be integrated using 2D fast Fourier transform. Using fast Fourier transform has the accuracy and speed advantage compared with finite-difference methods. Hopf instability leads to homogeneous oscillations, spatiotemporal chaos and spiral waves [1] similar to Belousov-Zhabotinsky chemical waves. In the case of Wave instability, the direct numerical simulation showed that spatiotemporal (periodic, quasi-periodic, or chaotic) modulation of the uniform profile is formed. Characteristic sizes of excited pattern are in good agreement with analytical predictions. Nonlinear interaction of four travelling waves forms the square optical vortex lattice similar to vortex lattices observed in superconductors and Bose Einstein condensate.

Acknowledgements.

The study was supported in part by the Ministry of education and science of Russia under Competitiveness Enhancement Program of SSAU for 2013-2020 years and by State assignment to educational and research institutions under projects 1451, GR 114091840046, by RFBR under grant 16-32-60151 mol_a_dk

References

[1] Anchikov D.A., Krents A.A., Molevich N.E., Pakhomov A.V. (2014) Dynamic modes of wide-aperture laser systems above the second lasing threshold. *Bulletin of the Lebedev Physics Institute*, Vol. 41, Iss. 8, pp. 226–229.

Improvement of error bound for dot product with unit in the first place

Katsuhisa Ozaki

Department of Mathematical Sciences, Shibaura Institute of Technology, Fukasaku 307, Minuma-ku, Saitama-shi, Saitama 337-8570, Japan
ozaki@sic.shibaura-it.ac.jp

Keywords. floating-point arithmetic ; rounding error estimation; numerical linear algebra.

This talk is concerned with rounding error estimation for dot product by numerical computations. Dot product is one of basic computations in numerical linear algebra. We use floating-point numbers and floating-point arithmetic as defined by the IEEE 754 standard [1]. Topics of error bounds for summation and dot product are summarized in chapters 3 and 4 in [2]. Recently, Rump and Jeannerod improved the error estimation of summation and dot product [3].

Rump proposed new type of error bounds for summation and dot product by using unit in the first place of floating-point numbers [4]. Let n and u be length of vectors and unit roundoff, respectively. If $(n+2)u \leq 1$, then a constant depending on n and u of the error bound for dot product by Rump is $(n+2)u$.

Our aim is to improve the error estimation of the dot product with unit in the last place by Rump. For $n = 2$ we succeed to derive the optimal constant $(2.5 - u)u$ for the error bound. Next, we proved that the constant for the error bound can be reduced to $(n + 1)u$ for $n \leq 25$ for binary32 and $n \leq 54$ for binary64 . Finally, error bound for arbitrary n could be derived.

Acknowledgments.

This research was supported by JSPS KAKENHI Grant Number 25730076.

References

[1] ANSI/IEEE 754-2008 (2008), *IEEE Standard for Floating-Point Arithmetic*, IEEE, New York.

[2] Higham N. J. (2002) *Accuracy and Stability of Numerical Algorithms, Second Edition*. SIAM, Philadelphia.

[3] Jeannerod C.-P. and Rump S.M. (2013) Improved error bounds for inner products in floating-point arithmetic. *SIAM. J. Matrix Anal. & Appl. (SIMAX)*, Vol. 34, pp. 338–344.

[4] Rump S.M. (2012) Error estimation of floating-point summation and dot product. *BIT Numerical Mathematics*, Vol. 52, pp. 201–220.

Numerical simulation of precessing vortex core dumping by localized nonstationary heat source

Denis Porfiriev 1, Anastasiya Gorbunova 1, Igor Zavershinsky 1, Semen Sugak 1, Nonna Molevich 2

1 Samara State Aerospace University, Samara, Russia
2 Lebedev Physical Institute, Samara, Russia
dporfirev@gmail.com

Keywords. Swirling flow; numerical simulation; precessing vortex core.

The precessing vortex core (PVC) appearance in technical devices with the heat release requires a thorough physical understanding of the influence of heat release on parameters of swirling flows. For this purpose, we performed the 3D numerical simulations of PVC in the swirling flow created in the open tube with the paraxial nonstationary heat source. Power of the source was modulated by sinusoidal law. We showed that three turbulence models give the qualitatively similar dependences of PVC frequency and amplitude on the heat-source power. The numerical simulation demonstrated that the obtained PVC is the left-handed co-rotated bending single-vortex structure. For considered values of the swirl and mass flow rate, we obtained that, for wide range of modulation frequencies, the growth of the heat-source power leads to gradual increase in the PVC frequency and slow change in the amplitude of vortex core oscillations. However, for specific modulation frequency, which depends on the tube geometry, dependencies of the PVC frequency and the amplitudes of oscillations have distinct maximum and minimum. Which means that, under specific conditions, flow pattern changes dramatically and precession is almost dumped at the relatively low values of heat power.

Acknowledgements.

The study was supported by The Ministry of education and science of Russia through Competitiveness Enhancement Program 2013-2020, by State assignment to educational and research institutions through projects 102, 608.

Steffensen's Method for Approximating Roots of p-Adic Polynomial Equations

Julius Fergy T. Rabago, Jerico B. Bacani

Department of Mathematics and Computer Science
College of Science
University of the Philippines Baguio
Baguio City 2600, Benguet, Philippines
jfrabago@gmail.com, jicderivative@yahoo.com

Keywords. Steffensen's method; Hensel's lemma; p-adic polynomials; p-adic numbers; roots of polynomials.

The notion of p-adic numbers was introduced by Kurt Hensel in 1897. This paves the way to the construction of the field of p-adic numbers $\mathbb{Q}_p$ as a completion of $\mathbb{Q}$, radically different from the field of real numbers. Since then, various applications of these numbers to different fields of mathematics and related areas in the applied sciences have been proposed and discovered. Meanwhile, Hensel's lemma plays a significant part in the study of this field including especially the field of p-adic integers $\mathbb{Z}_p$ by providing sufficient conditions for the existence of roots in $\mathbb{Z}_p$ of polynomials in $\mathbb{Z}_p[x]$. A classical application of this lemma deals with the problem of finding roots of a p-adic number a in $\mathbb{Q}_p$. Regarding this, Knapp and Xenophontos [3] showed how classical root-finding methods from numerical analysis can be used to calculate inverses of units modulo prime powers. A similar problem was also examined in [4] wherein Zerzaihi and Kecies considered the problem of finding the cubic roots of p-adic numbers in $\mathbb{Q}_p$ using Newton's method. We mention that none of these investigations gave account to the problem of finding roots of a general p-adic polynomial in $\mathbb{Z}_p$. Motivated by this remark and by the aforementioned works, we propose an analogue of Steffensen's method in finding roots of a general polynomial equation $f(x) = 0$ in $\mathbb{Z}_p[x]$ – thereby providing a generalization of previous investigations regarding root-finding problems in the p-adic setting.

References

[1] Dahlquist G., Björck A. (1974) *Numerical Methods*. Prentice-Hall, Englewood Cliffs.

[2] Katok S. (2007) *p-Adic Analysis Compared with Real*. Student Mathematical Library, Vol. 37, American Mathematical Society.

[3] Knapp M., Xenophontos C. (2010) Numerical Analysis meets Number Theory: Using root finding methods to calculate inverses mod p^n, *Appl. Anal. Discrete Math.*, Vol. 4, pp. 23–31.

[4] Zerzaihi T., Kecies M. (2013) General approach of the root of a p-adic number. *Filomat*, Vol. 27., No. 3, pp. 431–436.

An efficient gradient-based method for differential-interference-contrast microscopy

Simone Rebegoldi, Lola Bautista, Marco Prato, Luca Zanni, Laure Blanc-Féraud, Arturo Plata

Università di Modena e Reggio Emilia, Via Campi 213/B, Modena, Italy
Universidad Industrial de Santander, 680002 Bucaramanga, Colombia
Université Nice Sophia Antipolis, 06903 Sophia Antipolis, France
simone.rebegoldi@unimore.it, bautista@i3s.unice.fr,
marco.prato@unimore.it, luca.zanni@unimore.it,
laure.blanc_feraud@inria.fr, aplatag@yahoo.com

Keywords. DIC microscopy; inverse problems; gradient-descent method.

Differential-interference-contrast (DIC) microscopy is an optical microscopy technique widely used in biology to observe unstained transparent specimens, in which a two-dimensional image is formed from the interference of two waves that have a lateral differential displacement (shear) and are phase shifted relative one to each other. Following the rotational-diversity model proposed in [1], one is interested in retrieving the specimen's phase function from a set of DIC intensity images acquired at different rotations of the specimen. This highly nonlinear, ill-posed problem is solved by adopting a least squares approach and thus looking for a regularized solution of a smooth nonconvex optimization problem.
As already done in [1], one can address the DIC problem by means of a nonlinear conjugate gradient method, which is particularly suited for least squares problems. However, the computation of the line search parameter at each iteration may require several evaluations of both the function and its gradient in order to ensure convergence [2], which significantly increases computational time when such evaluations are time-consuming, as is the case of the DIC problem.
In this light we propose an efficient gradient-descent method for the estimation of a specimen's phase function from polychromatic DIC images. The method minimizes the sum of a nonlinear least-squares discrepancy measure and a smooth approximation of the total variation and exploits a recent updating rule for the choice of the step size [3]. Numerical simulations on two computer-generated objects show significant improvements in terms of efficiency and stability with respect to widely used conjugate gradient methods.

References

[1] Preza C. (2000) Rotational-diversity phase estimation from differential interference contrast microscopy images. J. Opt. Soc. Am. A, Vol. 17, no. 3, pp. 415–424.
[2] J. C. Gilbert, J. Nocedal. (1992) Global convergence properties of conjugate gradient methods for optimization. SIAM J. Optim., Vol. 2, No. 1, pp. 21–42.
[3] R. Fletcher. (2012) A limited memory steepest descent method. Math. Program., Vol. 135, No. 1–2, pp. 413–436.

Supertasks and Numeral Systems

Davide Rizza

University of East Anglia, School of Politics, Philosophy, Languages and Communication, Norwich, NR4 7TJ, United Kingdom
d.rizza@uea.ac.uk

Keywords. supertasks; paradox; grossone.

A supertask consists of an actual infinity of individual tasks, which can be carried out sequentially to completion in a finite amount of time. The recent philosophical literature has produced several paradoxes supported by a supertask scenario. Physical supertasks (e.g. [3]) have been invoked to show that certain counterintuitive consequences (e.g. self-excitation of a mechanical system, action without interaction) are compatible with classical or relativistic mechanics. Decision-theoretic supertasks have been used to construct sequences of rational choices that are irrational in the limit (e.g. [2]) or games that, even if they can be won under finitely many repetitions, fail to have a winning strategy in the limit [1]. Supertasks are standardly represented by a sequence of individual tasks, whose labels $1, 2, 3, \ldots$ are supplied by a traditional numeral system (e.g. in base ten). These labels cannot represent a sequential, completed infinity: they only sustain limit arguments, which rely on potential infinity. The work of Yaroslav Sergeyev on the grossone methodology shows that completion and sequential form are only incompatible as a result of the limited expressive power of the numeral system employed. Incompatibility is naturally overcome through the introduction of Sergeyev's numeral system, which gives rise to a representation of the set of natural numbers as a terminating sequence. When this representation is available, every supertask can be studied as an actually infinite, terminating process and its resolution is computable by elementary means. Moreover, the computable resolution shows that what appeared as existence problems (e.g. the existence of a physical state, a winning strategy etc.) under weaker numeral systems are in fact to be regarded as indexing problems, whose resolution is carried out through the introduction of a stronger numeral system.

References

[1] Bacon, A. (2010) A paradox for supertask decision makers. *Philosophical Studies*,Vol. 153, pp. 307–311.

[2] Barrett, J.F. and F. Arntzenius (1999) An infinite decision puzzle. *Theory and Decision*, Vol. 46, pp. 101–103.

[3] Laraudogoitia, J.P. (2009) Physical action without interaction. *Erkenntnis*, Vol. 70, pp. 365–377.

[4] Sergeyev, Ya. D. (2003) *The Arithmetic of Infinity*. Edizioni Orizzonti Meridionali, Rende.

An upper J- Hessenberg reduction of a matrix through symplectic Householder transformations

Ahmed Salam, Haitem Ben Kahla

University Lille Nord de France, ULCO, LMPA, BP 699, F62228, Calais, Cedex, France
University of Tunis E l Manar, ENIT-LAMSIN, BP 37, 1002, Tunis, Tunisia.
salam@lmpa.univ-littoral.fr, benkahla@lmpa.univ-littoral.fr

Keywords. Structured matrices; structure-preserving eigenproblems ; symplectic Householder transformations ; SR decomposition ; upper J- Hessenberg form.

In this talk, we derive a reduction of a matrix to a condensed form, the upper J- Hessenberg form, via elementary symplectic Householder transformations, which are rank-one modification of the identity . Features of the reduction are highlighted. Also, we give the implicit S theorem, which is the analog of the implicit Q theorem, when instead of the QR iteration, the SR iteration is used. Some numerical experiments of the reduction showing its efficiency are given.

References

[1] A. Salam, A. El Farouk, E. Al-Aidarous, Symplectic Householder Transformations for a QR-like decomposition, a Geometric and Algebraic Approaches, J. of Comput. and Appl. Math., Vol. 214, Issue 2, 1 May 2008, Pages 533-548.

[2] A. Salam and E. Al-Aidarous and A. Elfarouk, Optimal symplectic Householder transformations for SR-decomposition, Linear Algebra and Its Appl., 429 (2008), no. 5-6, 1334-1353.

[3] A. Salam and E. Al-Aidarous, Equivalence between modified symplectic Gram-Schmidt and Householder SR algorithms, BIT Numer. Math., Vol. 54, pp. 283-302, 2014.

A finite integration method for Boundary Value ODEs

Teerapol Saleewong1, Chamaiporn Cotnam2 and Sayaphat Susai3

1 Departmen of Mathematics, Faculty of Science, King Mongkuts University of Thonburi, Bangkok, Thailand.
2 Departmen of Mathematics, Faculty of Science, King Mongkuts University of Thonburi, Bangkok, Thailand.
3 Department of Mathematics, Facculty of Science, Srinakarinwirot University, Bangkok, Thailand.
teerapol.sal@kmutt.ac.th, chamaiporn.tuk@mail.kmutt.ac.th and sirirats@swu.ac.th

Keywords. Basis function; Finite integration method; Integration matrix

We propose a finite integration method with basis function for solving the differential equations. The integration matrix of the first order is obtained by the direct integration with either linear approximation or basis functions. Based on this matrix, any finite integration matrix with multi-layer integration can be obtained directly by the use of the matrix of first order. To compare numerical of this methods, the finite difference method are used. The finite integration method is extended to solve ordinary differential equation by transform technique. The solution is obtained suitable selection of the free parameters, the numerical examples demonstrate the accuracy and efficiency of the proposed method

Fuzzy Ensemble based Data Fusion in A Big Data Environment

Jiwan Seo, Seungjin Choi, Junho Kim, Sangyong Han

Department of computer science Engineering, Chungang Univ., Heukseok-dong, Dongjak-gu, Seoul, Korea
(jwseo, bethemoney, taki0112)@ec.cse.cau.ac.kr, hansy@cau.ac.kr

Keywords. Big data ; Ensemble ; Fuzzy; Decision support.

In a complicated application system, many different types of data are collected. Each of these data sets shows a different spatial and temporal degree so a simple combination would lead to the erroneous results. Therefore, data fusion is used to bring all data and attributes into a single view in which a more complete solution of the problem is created. In a big data environment, data sources are more diverse and usefulness of collected data also vary considerably. It has become necessary for information systems to be able to evaluate the usefulness of collected data as some of them are just a noise.

In this paper, we propose a fuzzy-ensemble machine learning-based evaluation method which would assess the usefulness of data collected from various sources. The proposed model has three modules to deduce the usefulness. One is the ensemble module that is composed of varying association analyzers for finding the relationship between the data and goal; the second module is a fuzzy module for interpreting and combining the results that are derived from the ensemble module; and the other module is an analysis/prediction module to achieve the objects of the system.

Using the proposed method, we can quantify the degree of usefulness and compare the usefulness of data in relation to other data. We verified the relationship between the calculated usefulness and the goal of a system by using real-world data to evaluate the proposed method; for this, we calculated the usefulness by using association-rule-based ensemble analyzers and the performance of a real-world, data-based movie recommendation system. As a result, we proved the correlation between usefulness and performance for the evaluation of our proposed method.

Acknowledgements.

This research was supported by the Chung-Ang University Research Scholarship Grants in 2015 and this research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Science, ICT and future Planning (NRF - 2015R1A2 A2A01005304)

Acceleration Techniques in the Univariate Lipschitz Global Optimization

Yaroslav D. Sergeyev, Dmitri E. Kvasov, Marat S. Mukhametzhanov

University of Calabria, Via Pietro Bucci 42C, 87036 Rende (CS), Italy
Lobachevsky State University, Gagarin Av. 23, 603950 Nizhni Novgorod, Russia
{yaro,kvadim,marat}@dimes.unical.it

Keywords. Lipschitz Global optimization; univariate problems; operational characteristics

Univariate box-constrained global optimization problems are considered in this contribution. The objective function is supposed to be "black-box", multi-extremal, non-differentiable, and hard to evaluate. Furthermore, the objective function is supposed to satisfy the Lipschitz condition over the search interval. Geometric and information statistical approaches are presented. The novel powerful local tuning and local improvement techniques are described in the contribution as well as the traditional ways to estimate the Lipschitz constant. The advantages of the presented local tuning and local improvement techniques are demonstrated using the operational characteristics approach for comparing deterministic global optimization algorithms on the class of 100 widely used test functions.

Acknowledgements.

This work was supported by the project No. 15-11-30022 "Global optimization, supercomputing computations, and applications" of the Russian Science Foundation.

References

[1] Ya. D. Sergeyev, M. S. Mukhametzhanov, D. E. Kvasov, and D. Lera (2016), Derivative-free local tuning and local improvement techniques embedded in the univariate global optimization, *Journal of Optimization Theory and Applications*, in Press.

[2] Ya. D. Sergeyev and D. E. Kvasov and M. S. Mukhametzhanov (2016), Operational zones for comparing metaheuristic and deterministic one-dimensional global optimization algorithms,*Mathematics and Computers in Simulation*, In Press.

[3] D. E. Kvasov and M. S. Mukhametzhanov and Ya. D. Sergeyev (2014), A numerical comparison of some deterministic and nature-inspired algorithms for black-box global optimization, in Proceedings of the *Twelfth International Conference on Computational Structures Technology* (ed. by B. H. V. Topping and P. Iványi), Naples (Italy).

[4] Ya. D. Sergeyev and D. E. Kvasov and M. S. Mukhametzhanov (2016), Comments upon the Usage of Derivatives in Lipschitz Global Optimization, in Proceedings of the *ICNAAM 2015: 13th International Conference of Numerical Analysis and Applied Mathematics*, Rhodes (Greece), In Press.

Inverse Scattering Problems for the Perturbed Biharmonic Operator

Valery Serov

University of Oulu, Finland valeri.serov@oulu.fi

Keywords. Biharmonic operator; Inverse scattering; Born approximation.

Some inverse scattering problems for operator of order 4 which is the perturbation (in smaller terms) of the biharmonic operator in one and three dimensions are considered. The coefficients of this perturbation are assumed to be from some Sobolev spaces (they might be singular). The classical (as for the Schrödinger operator) scattering theory (see, for example, [1]) is developed for this operator of order 4. The classical inverse scattering problems are considered and their uniqueness is proved. The method of inverse scattering Born approximation (see [2]) and an analog of Saito's formula (see, for example, [3]) are justified for this operator of order 4. Using this approximate method the reconstruction of the singularities of the unknown coefficients is proved in the scale of Sobolev spaces (see, for example, [4]). The results have natural generalization for any dimensions.

References

[1] Agmon S. (1975) Spectral properties of Schrödinger operators and scattering theory. *Ann. Scuola Norm. Sup. Pisa*, Vol. 2, pp. 151–218.

[2] Päivärinta L., Somersalo E. (1991) Inversion of discontinuities for the Schrödinger equation in three dimensions. *SIAM J. Math. Anal.*, Vol. 22, pp. 480–499.

[3] Päivärinta L., Serov V. (1998) Recovery of singularities of a multi-dimensional scattering potential, *SIAM J. Math. Anal.*, Vol. 29, pp. 697–711.

[4] Bergh J., Löfström (1976) *Interpolation spaces: An introduction.* Springer-Verlag, New York.

Acceptance Tail Ziggurat Algorithm for Generating Unimodal Random Variables

Efraim Shmerling

Ariel University,Science Park,44837 Ariel,Israel
efraimsh@ariel.ac.il, efraimsh@yahoo.com

Keywords. Random number generation; algorithm;unimodal random variable

A new algorithm for generating a random variable (rv) X with an unbounded range R and continuous unimodal probability density function (pdf) f(x) is presented. It is widely accepted that if f is decreasing or symmetric ziggurat algorithm [1] is the fastest of the algorithms that can be implied for sampling from the distribution in terms of generation time. However, ziggurat algorithm requires generation of tables at the preliminary setup stage which is time-expensive. Due to this drawback ziggurat has never been considered a viable option for most widely applied rv's. We have developed an algorithm named exceptance tail(AT) ziggurat equally efficient to ziggurat in terms of generation time, requiring significantly less time for generating the tables. It can be recommended as a instrument for sampling from many widely applied distributions.It is based on covering the "bulk" of the density region by equi-area horizontal rectangles as is the case in ziggurat, and implements a universal AT method for generating rv's which significantly differs from the "classical" acceptance rejection method implied in ziggurat. The version of the AT method for generating a continuous univariate rv X with an unbounded range R is introduced. At the setup stage R is divided into 2 parts: a bounded interval C and an unbounded domain $T = R - C$. Let H designate the part of the density region over C. A set of non-intersecting equi-area rectangles with total area 1 covering H has to be found. In order to generate X, we select a rectangle indexed i, which extends from $l(i)$ to $r(i)$ horizontally and from $b(i)$ to $c(i)$ vertically, generate a random point x uniformly distributed in $(l(i); r(i))$. If x satisfies the inequality $b(i) + y < f(x)$, where y is sampled from a uniform distribution in $(b(i), c(i))$, we set $X = x$; otherwise, generate G with pdf: $g(x) = f(x)/(1 - A(H))$, $x \in T$.

References

[1] Marsaglia, G. and Tsang, W. W. 2000. The ziggurat method for generating random variables. Journal of Statistical Software 5, 17. www.jstatsoft.org.

Discussion of a new iterative algorithm for numerical reckoning fixed points of Suzuki's generalized nonexpansive mappings

Wutiphol Sintunavarat[1], Adoon Pansuwan[1]

[1]Department of Mathematics and Statistics, Faculty of Science and Technology, Thammasat University Rangsit Center, Pathumthani 12121, Thailand.
wutiphol@mathstat.sci.tu.ac.th, pansuwan@mathstat.sci.tu.ac.th

Keywords. Fixed points; Suzuki's generalized nonexpansive mappings; Uniformly convex Banach spaces.

The aim of this work is to propose a new iterative algorithm to approximate fixed point of Suzuki's generalized nonexpansive mappings. We prove some weak and strong convergence theorems in uniformly convex Banach spaces and also provide an example of a Suzuki's generalized nonexpansive mapping and numerically compare the convergence of the purposed iteration with the method of successive substitution (Picard iteration) and the well-known Mann's iteration, Ishikawa's iteration, Noor's iteration and the recent iterations of Agarwal et al. [1], Abbas et al. [2] and Thakur et al. [3].

Acknowledgements.

This research was supported by Thammasat University under the TU Research Scholar, Contract No. 2/8/2558.

References

[1] Agarwal R.P., O'Regan D., Sahu D.R. (2007) Iterative construction of fixed points of nearly asymptotically nonexpansive mappings. *J. Nonlinear Convex Anal.* Vol. 8, pp. 61–79.

[2] Abbas M., Nazir T. (2014) A new faster iteration process applied to constrained minimization and feasibility problems. *Mat. Vesn.*, Vol. 66, pp. 223–234.

[3] Thakur B.S., Thakur B., Postolache M. (2016) A new iterative scheme for numerical reckoning fixed points of Suzuki's generalized nonexpansive mappings. *Appl. Math. Comput.* Vol. 275, pp. 147–155.

Automatic discovery of the communication network topology for building a supercomputer model

Sergey Sobolev, Konstantin Stefanov, Vadim Voevodin

RCC MSU, Moscow, Leninskie gory, 1, bld. 4, Russia
{sergeys,cstef,vadim}@parallel.ru

Keywords. Supercomputer; topology discovery; Infiniband; Ethernet.

RCC MSU is developing the Octotron system [1] which is designed to automatically detect and eliminate consequences of emergency situations in supercomputers in order to maximize the safety of equipment and minimize resource downtime. This system is based on a supercomputer model that describes the components of the computing system and their interconnections. Octotron constantly compares the "theory" (model description) and the "practice" (real monitoring data) and reacts accordingly if they differ.

The quality of the Octotron service heavily depends on the completeness of the model. Since its very difficult to create such model manually, this process should be automated. One of the main supercomputer components is the communication network, so it was decided to develop a tool for automatic model detection and description for Infiniband and Ethernet networks in supercomputing systems.

This tool automatically detects nodes and switches, collects needed description data and identifies connections between them. ARP data, forwarding tables and LLDP protocol results are used to build the Ethernet network topology; data from subnet manager is used for the Infiniband network. The distinctive features of this tool are: detection of both switches and computing nodes; flexibility of the data to be collected; intellectual identification of the objects and interconnects that were not identified directly; open source. At the moment the tool has been successfully used as part of the Octotron system installed on the largest Russian supercomputer systems.

Acknowledgements.
This work is supported by RFBR, research project No. 16-07-01199.

References

[1] Antonov A., Nikitenko D., Shvets P., Sobolev S., Stefanov K., Voevodin Vad., Voevodin V. and Zhumatiy S.: An Approach for Ensuring Reliable Functioning of a Supercomputer Based on a Formal Model. LNCS 9573 (accepted).

The Minimum Norm Least Squares Solution to the Discrete Nonlocal Problems

Artūras Štikonas, Gailė Paukštaitė

Vilnius University, Akademijos 4, LT-08663 Vilnius, Lithuania
Vilnius University, Naugarduko 24, LT-03225 Vilnius, Lithuania
arturas.stikonas@mif.vu.lt, gaile.paukstaite@mif.vu.lt

Keywords. Discrete problem; Generalized Green's function; Least squares solution; Moore–Penrose inverse.

We consider the second order differential problem with two linear nonlocal conditions and take a discrete representation of the differential problem.

Firstly, we introduce two finite dimensional Hilbert spaces. The general solution, that minimizes the residual of the discrete problem in the norm of the first Hilbert space, provides the one solution of the minimum norm of the second Hilbert space. We investigate the properties of this solution. Moreover, generalized Green's function, describing this solution as ordinary Green's function describes the unique exact solution, is analyzed also. Its properties are presented as well.

Secondly, applying the properties of this solution and generalized Green's function, we analyze if the minimum norm least squares solution converges to the minimum norm least squares solutions of the differential problem. We answer the question: what particular norms have to be chosen to the discrete problem? The sufficient conditions for the convergence are also discussed. Finally, we give a few examples that illustrate the results obtained.

Acknowledgements.
This research was supported by the Research Council of Lithuania (grant No. MIP-047/2014).

References

[1] Ben-Israel A., Greville T.N.E. (2003) *Generalized Inverses. Theory and Applications*. Springer Verlag, New York.

[2] Paukštaitė G., Štikonas A. (2015) Ordinary and generalized Green's functions for the second order discrete nonlocal problems. *Bound. Value Probl.*, Vol. 2015:207, pp. 1–19.

[3] Penrose R. (1956) On best approximate solutions of linear matrix equations. *Proc. Cambridge Philos. Soc.*, Vol. 52, pp. 17–19.

[4] Štikonas A., Roman S. (2009) Stationary problems with two additional conditions and formulae for Green's functions. *Numer. Funct. Anal. Optim.*, Vol. 30(9), pp. 1125–1144.

Modeling of the Non-Steady Navier-Stokes Equations in Thin Structures

Olga Štikonienė

Vilnius University, Vilnius, Lithuania
olga.stikoniene@mif.vu.lt

Keywords. Navier-Stokes equations; thin structures; multiscale models.

The method of asymptotic partial domain decomposition for thin tube structures (finite unions of thin cylinders) was developed in [1, 2]. Thin structures are some finite unions of thin rectangles (in $2D$ settings) or cylinders (in 3D settings) depending on small parameter that is, the ratio of the thickness of the rectangle (cylinder) to its length. The Navier–Stokes equations are considered in thin structures with the no-slip boundary condition at the lateral boundary and with the inflow and outflow conditions with the given velocity. I report computer simulations of flows in 2D tube systems. I will discuss details of numerical approach and some technical aspects of asymptotic analysis.

This is a joint work with G. Panasenko and K. Pileckas.

Acknowledgements.

This research was supported by the Lithuanian-Swiss cooperation programme to reduce economic and social disparities within the enlarged European Union under project agreement No. CH-3-SMM-01/01.

References

[1] Panasenko G., Pileckas K. (2015) Asymptotic analysis of the non-steady Navier-Stokes equations in a tube structure. I. The case without boundary layer-in-time, *Nonlinear Analysis, Series A, Theory, Methods and Applications*. Vol. 122, pp. 125–168.

[2] Panasenko G., Pileckas K. (2015) Asymptotic analysis of the non-steady Navier-Stokes equations in a tube structure. II. General case, *Nonlinear Analysis, Series A, Theory, Methods and Applications*. Vol. 125, pp. 582–607.

Approximating a Nonlinear Advanced-Delayed Equation From Acoustics

M. Filomena Teodoro

CEMAT, Instituto Superior Técnico, Av. Rovisco Pais,1, 1094-001 Lisboa, Portugal
CINAV, Portuguese Naval Academy, Base Naval de Lisboa, Alfeite, 1910-001 Almada, Portugal
maria.alves.teodoro@marinha.pt

Keywords. Numerical Approximation; Forward-Backward Equation; Nonlinear; HAM.

The aim of this article is to solve numerically a mathematical equation which models a superficial wave propagating through the tissues. It is developed a numerical scheme which approximates the solution of a particular nonlinear mixed type functional differential equation from acoustics. We compare the computed results with a recent numerical approximation obtained by a scheme based on Newton method, collocation and method of steps. Two different approaches are taken into account, when there are considered a small time delay and an arbitrary time delay.

Acknowledgements.

This work was supported by Portuguese funds, *The Portuguese Foundation for Science and Technology* (FCT), through the *Center for Computational and Stochastic Mathematics* (CEMAT), University of Lisbon, Portugal, project UID/Multi/04621/2013, and *Center of Naval Research* (CINAV), Naval Academy, Portuguese Navy, Portugal.

Discretization of the Schwarzian Derivative

Toshiaki Itoh

Doshisha University of Kyoto, Japan
toito@mail.doshisha.ac.jp

Keywords. Schwarzian Derivative; Discretization; Conformal mapping.

The Schwarzian derivative is old topics, but it appears often in many research areas even now. For example, the interest of discretization of analytically integrable or geometrical system sometimes leads us to the Schwarzian derivative. There were many works about the Schwarzian derivative already. Therefore at the beginning in this study, we review the correspondence between the Schwarzian derivative and the Cross-ratio, then consider their application.

As an example, we apply discretized Schwarzian derivative to conformal mapping. It is well known that the Schwarzian derivative gives conformal mapping from upper half plane of complex space to inside of multi-arc polygon. In this application, since discrete counterpart of the Schwarzian derivative is the Cross-ratio actually, we apply Cross-ratio to conformal mapping.

The problems of what we meet on such mapping with Cross-ratio are treatment of singularities of the mapping at the vertices of polygon and evaluation of accessary parameters. It found we can solve this by coming and going between the Schwarzian derivative and Cross-ratio. Moreover this approach leads us to the entrance of discrete integrable system of special functions from the classical treatment of 2nd order ODE and difference equations. Such discrete integrable system is composed of simultameous equation of the two Möbius trandformations or discrete Riccati's eqautions.

Acknowledgements.

I would like to express my gratitude to Numerical Analysis group of Mathematisches Institut, Universitat Tübingen in Germany for many assistance of my visiting and research.

References

[1] Ovsienko V., Yabachnikov S. (2009) What is ... the Schwarzian Derivative?. *Notices of the AMS*, Vol. 56, No. 1, pp. 34–36.

[2] Ttoh T. (2013) A Correspondence between Schwarzian derivative of ODE and Cross-ratio of ordinary difference equation. *AIP Conference Proceeding* Vol. 1558-1, pp. 2167.

[3] Ramani A., Gramaticos B., Tamizhmani T., Tamizhmani K. M. (2001) Special Function Solutions of the Discrete Painlevé Equations. *Compt. Math. Appl.*, Vol. 42, pp. 603–614.

Electrical simulating for chip formation process

Trofimov A., Sirotenko L., Khanov A., Losev V.

Perm national research polytechnical university, Perm, Komsomolsky prospect 29, Russian Federation
nameofmybox@mail.ru, mtf-dekanat@pstu.ru

Keywords. Dynamics process; chip formation; phenomena; edge cutting machining; mathematical simulation; direct analogy; equivalent element; numerical mathematical model; electric circuit; mechanic-hydro-electric model.

For science research of dynamics processes of chip formation phenomena, which observed in the edge cutting machining process, is used mathematical simulation method based on using of direct analogy models. Numerical mathematical model obtained by direct analogy method relates to the body of interests as a likeness but not an identity. Direct analogy models generates by electric circuit. For investigating complex phenomena by electrical simulating, model is generated and electrical processes are investigated. In this study mechanisms of machining parameters impacts to the surface quality are investigated. In this study chip formation process is presented as hydro-electrical interpretation edge cutting process, in other words hydraulic simulation first and then its electrical analogy. This way has chosen because dynamics of the chip formation process is easy to formulate through mathematical apparatus of circuit theory. As edge cutting process is considered as mechanical, hydraulic and electric system that its necessary to correlate each element of each system between each other so that its may be possible to show all investigated relations. As a result of this study mechanic-hydro-electric model is formed. Also the test problem for estimating the functionality of the method. Finding results makes is possible to estimate the mathematical model for efficiency and reliability, also makes it possible machining parameters optimization.

References

[1] Barbotko A. I. (2013) Basis of mathematical simulation, TNT, Stary Oskol.

Combination of Context-role and Perimeter Protection Paradigms for Modelling the Security of Information Systems

Hein Tun, Sergey Lupin, Aleksandr Gureev

National Research University of Electronic Technology, Zelenograd, Moscow, 124498, Russia
mr.heintun@gmail.com

Keywords. Hybrid modelling; estimation of security; information systems security.

A possibility of using the Hybrid Modelling for the estimation of information systems ability for preventing the unauthorized access has been analyzed. Proposed approach combines two paradigms of information security context-role and perimeter protection. AnyLogic was used as a platform for development and simulation the experimental model. AnyLogic allows us to use agent based and discrete event methods for formalization the processes in information systems security. According to the context-role model the permissions of agents are determined by their position in administrative hierarchy. In our approach the access rights of agents depend also from their position in protected environment. Article shows the structure of Anylogic model and set of data which provide the various behaviors of agents and the functionality of perimeter's protection. Simulation experiments confirmed the usability of hybrid models for estimation the level of information security. The set of agents parameters allows determining the wide range of their activities and investigating the reaction of security system to their behavior.

Acknowledgements. This article was prepared as part of the research project RFBR number 15-29-0795 "Dynamic sequential filling of telecommunication networks with centralized routing by communication flow for using in distributed systems".

References

[1] M. Nancylia, E.K Mudjtabar, S. Sutikno, and Y. Rosmansyah, "The measurement design of information security management system," in Proc. 2014 8th Int. Conf. on Telecommunication Systems Services and Applications, Kuta, Indonesia, 2014, pp. 15.

[2] Zhong Xiu-yu, "A model of online attack detection for computer forensics," in Proc. Int. Conf. on Computer Application and System Modeling, Taiyuan, China, 2010, vol. 8, pp. 533537.

[3] Wu Tianshui, and Zhao Gang, "A new security and privacy risk assessment model for information system considering influence relation of risk elements," in Proc. 2014 9th Int. Conf. on Broadband and Wireless Computing, Communication and Applications, Guangdong, China, 2014, pp. 233238.

[4] A. Bilbao, and E. Bilbao, "Measuring security," in Proc. 2013 47th Int. Carnahan Conference on Security Technology, Medellin, Colombia, 2013, pp. 15.

[5] Sergey Lupin, Hein Tun, Aye Min Thike, Mikhail Puschin, "Hybrid Modelling as a Tool for the Analysis of the Information Systems Security" In Proceedings of 2016 IEEE NW Russia Young Researches in Electrical and Electronic Engineering Conference (EIConRusNW) St. Petersburg, Russia, February 2 - 4, 2016.

Data mining method for anomaly detection in the supercomputer task flow

Denis Shaikhislamov, Vadim Voevodin, Vladimir Voevodin

RCC MSU, Moscow, Leninskie gory, 1, bld. 4, Russia
sdenis1995@gmail.com, vadim@parallel.ru, voevodin@parallel.ru

Keywords. Supercomputer; anomaly detection; task flow; program efficiency; data mining.

One of the most urgent and actual problems in high performance computing is the extremely low efficiency of supercomputer applications. The situation is complicated by the fact that in most cases users do not even know that their applications are not working efficiently. Therefore, special approach is needed to analyze the state of the entire supercomputer that allows detecting such inefficient applications.

A possible way to deal with this issue is to study a flow of tasks that run on a supercomputer in order to detect applications with unusual dynamic characteristics or activity (e.g., very low memory usage or deadlocks), in other words, applications with abnormal behavior.

In this paper we propose a new intelligent algorithm for detecting such anomalies in the supercomputer task flow. It is based on data mining methods and is designed as follows. Using system monitoring data, mean and spread of values for dynamic characteristics (such as CPU load, number of cache misses per second, Infiniband network load) is computed for each completed task. This data is used as an input for decision trees classification algorithm that assigns a task to a particular class. At the moment, each task can be one of three classes normal, suspicious and abnormal; in the future it is planned to separate different anomaly classes. Current results show that a surprisingly large percentage of tasks have an abnormally low resource usage.

Also in this paper we will show how different characteristics influence the choice of classification classes, which will help to determine the root causes of program anomaly behavior. The results will be demonstrated on the actual data from the Lomonosov supercomputer (1.7 PFlops peak, 5000 nodes, 500 completed tasks per day).

Acknowledgements.
This work is supported by RFBR, research project No. 16-07-00972.

A parallel approach for image segmentation by numerical minimization of a second-order functional

Riccardo Zanella, Massimo Zanetti, Valeria Ruggiero

Mathematics and Computer Science Dept., University of Ferrara, Ferrara, Italy
Information and Comm. Technology Dept., University of Trento, Trento, Italy
{riccardo.zanella,valeria.ruggiero}@unife.it, massimo.zanetti@unitn.it

Keywords. Segmentation; Blake and Zisserman functional; domain decomposition; block coordinate descent methods; parallel interconnection rules.

In the framework of variational approaches for image segmentation problems, the Blake-Zisserman second-order model has been introduced with the aim of overcoming the limitations of the Mumford-Shah. Recently in [1], the numerical minimization of the variational approximation of the functional given by Ambrosio, Faina and March [2] has been addressed. The authors propose to use an efficient block-coordinate descent algorithm (BCDA) that exploits a compact matricial formulation of the objective functional and its decomposition into quadratic sparse strongly convex sub-problems. In order to enable the segmentation of large-size gridded data, such as full-scene images or Digital Surface Models (DSMs) [3], we propose to combine BCDA with a domain decomposition technique and a parallel interconnection rule among blocks of variables. The aim of this paper is to show that a simple tiling strategy enables us to treat large images even in a commodity multicore CPU, with no need of specific post-processing on tiles junctions. From the point of view of the performance, little computational effort is required to separate data in subdomains; thus we expect a negligible time spent in data partitioning and communications, when compared to time for solving each independent task. Numerical results will be provided in order to evaluate the effectiveness of the approach.

Acknowledgements: This research was supported by the following grants: INDAM-GNCS2016, FIRB2012 grant RBFR12M3AC

References

[1] M. Zanetti, V. Ruggiero, M. Miranda Jr. (2016) Numerical minimization of a second-order functional for image segmentation, *Commun. Nonlinear Sci. Numer. Simul.*, 36, 528–548.

[2] L. Ambrosio, L. Faina, R. March (2001) Variational approximation of a second order free discontinuity problem in computer vision, *SIAM J. Math. Anal.*, Vol. 32, No. 6, 1171–1197.

[3] M. Zanetti, A. Vitti (2013) The Blake-Zisserman model for digital surface models segmentation, *ISPRS Ann. Photogramm. Remote Sens. Spatial Inf. Sci.*, II-5/W2, 355–360.

Determining Evaporation in the Model of Water Transfer in Soil

Sergey Zasukhin

Moscow Institute of Physics and Technology, 9 Institutskiy pereulok, Dolgoprudny, Moscow region, 141700, Russia
s.zasukhin@yandex.ru

Keywords. Optimal control; evaporation; parabolic equation.

A model of vertical water transfer in soil is considered. Under the assumption that soil is an isothermal porous homogeneous medium, a process of vertical water transfer in soil can be described by one-dimensional nonlinear parabolic equation. The coefficient of diffusion and the hydraulic conductivity are expressed by the widely used formulas of van Genuchten [1].

Identification of soil hydraulic parameters was investigated by many authors (see, for example, [2]). Evaporation process is important for the water exchange between the atmosphere and the land surface and is widely used in climatology and hydrology. In the same time, evaporation is one of most hard-determined component of the model. In the research, a problem of determining evaporation is formulated as an optimal control problem. The objective function is mean-square deviation of soil moisture obtained by the model at various depths from some prescribed values. The sensitivity of soil moisture to changes of evaporation is estimated. These estimates allowed to determine an effective subsurface soil layer in which it is advisable to compare calculated values of soil moisture with prescribed ones and to compute the objective function. This region definition has accelerated the convergence of the optimization process and has reduced the time of its execution.

Acknowledgements.

This research was supported in part by the Russian Foundation of Basic Research under Grant 15-07-08952.

References

[1] Van Genuchten M. Th. (1980) A closed form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil. Sci. Soc. Am. J.*, Vol. 44, pp. 892–898.

[2] Durner W., Priesack E., Vogel H.-J., Zurmuhl T.(1999) Determination of parameters for flexible hydraulic functions by inverse modeling. In Proceedings of the *International Workshop on Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, Riverside, California October 22-24, 1997* (ed. by van Genuchten M. Th. and Leij F. J.), Riverside, California (USA), p. 817–829.

Decision Of Logical Equalizations By Recurrent Method

Kyaw Zaw Ye, A.A. Balabanov, L.G. Gagarina, E.M. Portnov, O.I. Lisov, V.A. Barhotkin

National Research University of Electronic Technology Russian Federation, 124498, Moscow, Zelenograd, 4806 passage, 5
kyawzawye85@gmail.com, gagar@bk.ru

Keywords. Logical equations; recurrent methods.

In this article the technique of the solution of the logical equations on the basis of drawing up recurrent ratios is described. The technique is effectively applicable to the logical equations and systems of the logical equations having uniformity of representation. The number of logic equations and systems of the logical equations are increasing in various test tasks for pupils recently. The complexity of equations is constantly increasing. However, in school textbooks, this section is a very meager. In recent publications necessary information appeared. In this article the authors examine the question of extending the sphere of application of one of the most effective methods for solving logic equations - recurrent method. The method is applicable to equations and systems that have structural homogeneity. The presentation is made on concrete examples from which are made imprecisely generalizations. Match of answers indicates the correctness of the solution according to one recurrent method. The considered problems confirm scope of recurrent method for solving logic equations. Separate equations and systems of logical equations must be structurally homogeneous. The authors hope that the material of the article will be useful for teachers of computer science, and students.

Theory for Typed Inclusion Dependencies with Null Values

Vladimir Zykin

Keywords. Inclusion dependencies; axiomatization; NULL values.

The paper deals with formal theory of typed inclusion dependencies (IND). These dependencies are widely applied in different papers, such in [1]. IND are used in designing of database schemes for organization of referential integrity constraint on data. The axiom system is presented with proof of soundness and completeness. Distinctive feature of axioms is possibility of using NULL values in IND. In practice it corresponds to incomplete or partial information in database. Special attention is given to original proof of axiom system completeness, which based on mathematical induction. Some arguments are taken into consideration about using of typed INDs in contrast to the untyped [2]. Formal theory is complemented by practical algorithm of typed INDs closure constraint. And on it base the algorithm of minimal cover construction is designed. These algorithms are polynomial-time such in [3].

Acknowledgements.

This research was supported by the Russian Foundation for Basic Research (project no.15-41-04436).

References

[1] Conforti R., Dumas M., Garcia-Banuelos L., La Rosa M. (2015) BPMN Miner: Automated Discovery of BPMN Process Models with Hierarchical Structure. Queensland University of Technology. Brisbane, Australia.

[2] Casanova M.A., Fagin R., Papadimitriou C.H. (1984) Inclusion Dependencies and Their Interaction with Functional Dependencies. JOURNAL OF COMPUTER AND SYSTEM SCIENCES Vol. 28, pp. 29–59.

[3] Missoui R., Godin R. (1990) The implication problem for Inclusion Dependencies: A graph approach. SIGMOD RECORD, Vol. 19, No. 1, pp. 36–40.

Complementarity Problem for the Stochastic Transportation Problem

Anna Zykina, Olga Kaneva, Tatiana Pavlyuchenko

Keywords. Complementarity problem; transportation problem; problem of stochastic programming.

In applications which used a classical transportation task

$$L(x) = \sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}x_{ij} \to \min,$$

$$\sum_{j=1}^{n} x_{ij} = a_i, \quad \sum_{i=1}^{m} x_{ij} = b_j, \quad x_{ij} \geq 0, \ i = 1, ..., m, \ j = 1, ..., n,$$

special attention is given to the stochastic formulation of the transportation problem [1]. It is usually assumed that the demand $b_j = b_j(\omega)$ in j-point of consumption is a random variable.

Let $z_j = \sum_{i=1}^{m} x_{ij}$ – is total volume of the product for consumption j. When condition $z_j \leq b_j(\omega)$ is true, the demand will not be satisfied. In this case there are additional costs according to short shipment of cargo. When $z_j \geq b_j(\omega)$, there are additional costs for excess product storage.

Transport problem with random demand can be turned to deterministic problem of convex programming with linear constraints. The objective function represents the mathematical expectation of total losses during transportation of the product, damages on poor demand and the costs of storing excess product.

However, not always such transformation gives an acceptable solution, so the need for other approaches to the problem is arised.

This article deals with a two-stage stochastic transport problem where the choice of compensation plan is a subject to the terms which are determined by a linear complementarity problem.

Acknowledgements.

This research was supported by the Russian Foundation for Basic Research (project no.15-41-04436)

References

[1] Judin D. B. (2010) *Mathematical methods of control under incomplete information. Objectives and methods of stochastic programming.* Krasand, Moscow.

Global Optimal Trajectory in Chaos and NP-Hardness

Vittorio Latorre[a], David Yang Gao[b]

[a]Department of Computer, Control and Management Engineering University of Rome Sapienza, Italy;
[b]School of Applied Sciences, Federation University Australia, Mt Helen, Victoria, 3353, Australia
latorre@dis.uniroma1.it, d.gao@federation.edu.au

Keywords. Chaos; NP-Hardness; Nonlinear Dynamics; Global Optimization; Canonical duality theory

We introduce an unconventional theory and method for solving general nonlinear dynamical systems. Instead of the direct iterative methods, the discretized nonlinear system is first formulated as a global optimization problem via the least squares method. A newly developed canonical duality theory shows that this nonconvex minimization problem can be solved deterministically in polynomial time if a global optimality condition is satisfied. The so-called pseudo-chaos produced by Runge-Kutta type of linear iterations are mainly due to the intrinsic numerical error accumulations. Otherwise, the global optimization problem could be NP-hard and the nonlinear system can be really chaotic. A conjecture is proposed, which reveals the connection between chaos in nonlinear dynamics and NP-hardness in computer science. The methodology and the conjecture are verified by applications to the well-known logistic equation, a forced memristive circuit and the Lorenz system. Computational results show that the canonical duality theory can be used to identify chaotic systems and to obtain realistic global optimal solutions in nonlinear dynamical systems. The presented method and results should bring some new insights into nonlinear dynamical systems and NP-hardness in computational complexity theory.