Characteristics of main research directions investigated at the institute and the achievements 2010−2014

Institute	Institute of Computer Science of the Czech Academy of Sciences

Introductory remarks

The list of research outputs submitted by the Institute of Computer Science for evaluation is quite colourful. To array them into a mosaic, a simple listing of research directions would not be sufficient.

Therefore, we offer a short tour of the institute, paying a brief visit to each of the seven teams, and highlighting their main achievements. The information from this section should be complemented by the subsequent sections 2–4. Without them, the mosaic would not be complete.

It should be emphasized at the outset that all teams subject to this evaluation exercise exist in their current form only from July 1, 2013. The reorganisation taking place at that date transformed four then existing departments into the current seven departments. Each department is one of the evaluated teams.

We shall not follow the organisational numbering of departments, but a route offering more comprehensible view of the institute.

The tour starts at Team 5, because it underwent an interesting development during the evaluated period, and it allows to illustrate traits important for understanding what has been taking place in the whole institute. The final of the tour is reserved for Team 1, because of its long-term sustained performance, and because it has followed a steady course with clearly articulated goals. We shall refer to it in Section 4.

A tour of teams, research directions, and achievements

1 Computational Methods
2 Theoretical Computer Science
3 Nonlinear Modelling
4 Medical Informatics and Biostatistics
5 Nonlinear Dynamics and Complex Systems
6 Optimization and Systems
7 Fundamental Topics

The development of **Team 5** is sketched in Fig. 1. Its kernel is the Nonlinear Dynamics Workgroup, whose founder, Milan Paluš, is one of the leading scientific personalities in the institute (h-index 23). He joined the institute as early as 1994 and his results gradually gained recognition. Thanks to a successful grant application in 2005 to the EC FP6, he was able to reinforce the group by hiring Martin Vejmelka, then a young cybernetics student with excellent programming skills. By the end of 2009, again thanks to funding from an EC FP7 project, the group was strengthened by Jaroslav Hlinka, who extended the team expertise in the analysis of electrophysiological data to the area of neurosciences. From his doctoral studies at the

University of Nottingham, UK, he brought the expertise in processing high dimensional neuroimaging data and in mathematical modelling of brain activity.

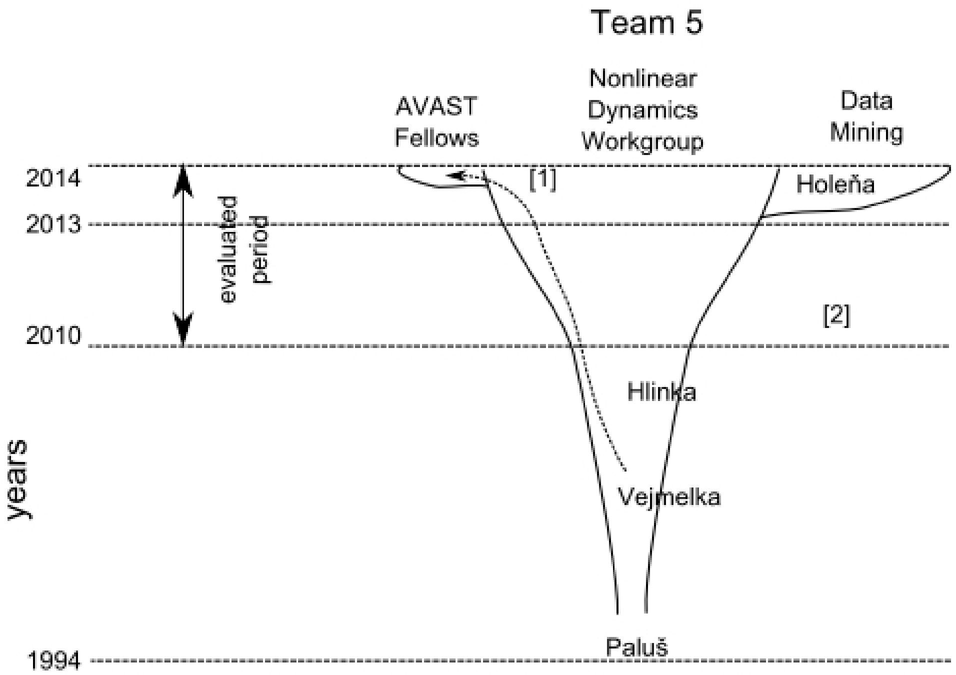


Fig. 1

During the evaluated period, the group grew in headcount as well as in the width of the themes studied. A remarkable example of recent scientific achievement of the group is

[1] M. Paluš: Multiscale atmospheric dynamics: Cross-frequency phase-amplitude coupling in the air temperature. *Physical Review. Letters.* 112, 078702, 2014.

In this paper, starting from long-time records of air temperature from various European cities, causality was discovered between eight-year temperature cycle and temperature variability in shorter time scale. The effect is quite significant - Prague records reveal changes of annual averages of about 1.5°C, in some areas of Germany and Poland the value reaches 2°C.

Fig. 1 indicates that the composition of the team was influenced by a reorganisation in mid-2013. The workgroup of nonlinear dynamics was joined by the group of Martin Holeňa, focused on data mining. Martin Holeňa, in cooperation with colleagues from several German research institutes, is interested in practical applications of data mining. Independently, he pursues also basic research in data mining. His first stream of research is illustrated by

[2] U. Zavyalova, **M. Holeňa,** R. Schlögl, M. Baerns: Statistical Analysis of Past Catalytic Data on Oxidative Methane Coupling for New Insights into the Composition of High-Performance Catalysts. *ChemCatChem* 3:1935–1947, 2011..

In addition, Fig. 1. captures quite recent development in 2014, when Martin Vejmelka, after a two year stint at the University of Colorado Denver, was awarded one of the two positions of AVAST Fellows created in cooperation with AVAST Software company (the second being Tomoyuki Suzuki). As early as six months after the commencement of their work, one of the ideas of Martin Vejmelka was cleared for production and the resulting method became a part of antivirus protection for more than 230 million computer users.

In Team 5 we have met two types of achievements we can recognize in a greater or lesser degree in other teams, in addition to published scientific results:

- *Development of an original method*: in this case the method enabling to discover causal relations in time series – method proven in the field of climatology as well as in brain studies.
- *Building of a team*.

1 Computational Methods
2 Theoretical Computer Science
3 Nonlinear Modelling
4 Medical Informatics and Biostatistics
5 Nonlinear Dynamics and Complex Systems
6 Optimization and Systems
7 Fundamental Topics

The development of **Team 4** resembles the previous team in its origin, however its story in the past 5 years is different. The origin of the team is also connected with a scientist joining the institute already in 1992 and gradually building a team – Jana Zvárová. Thanks to her organizational talent and fundraising abilities, she realized her plan to create a group able to offer applications of statistics and informatics to medical profession. In the context of educational activities and practical outputs, two directions of basic research emerged: application of biostatistics and reduction of complexity in high dimensional data. They dominate the work of the current department which took shape after financing of research center was finished and part of the workers focused mainly on the education of physicians and on practically oriented projects left the institute (here the story differs from the previous team).

An example of outcomes of the first direction – application of biostatistics – is the paper

[3] P. Kříž, M. Seydlová, T. Dostálová, **Z. Valenta,** K. Chleborád, **J. Zvárová,** J. Feberová, R. Hippmann: Dental implants and improvement of oral health-related quality of life. *Community Dentistry and Oral Epidemiology* 40:65–70, 2012.

The aim of this direction is to perform biostatistical analysis of data obtained in medical research, not only as a standard service provided for physicians, but in a close cooperation in which Team 4 participates in the design of medical experiments so that evidential conclusions can be reached.

The second direction aims at reduction of complexity in high dimensional data. Problems investigated in this direction differ from classical statistical tasks, where for each observation only a few measurements are at disposal. In medical studies, for example, there are typically a few clinical symptoms measured on hundreds of patients. On the contrary, in the area of high dimensional genetic data analysis, often thousands or tens of thousands variables are measured only on tens of patients.

This direction opened for the members of Team 4 thanks to an extensive study of genetic causes of myocardial infarction, realized in the past years by the research center in cooperation with several medical institutions. They obtained theoretical as well as practically oriented results, e. g. 4 national patents. An example of a theoretical work based on the results of the study, which was accepted for publication during the evaluated period is

[4] **Z. Valenta**, **J. Kalina**: Exploiting Stein's paradox in analysing sparse data from genome-wide association studies. *Biocybernetics and Biomedical Engineering* 35:64–67, 2015.

Team 7 differs somewhat from the other teams, reasons for it will be explained in Section 2. The team consists mostly of scientific personalities studying diverse topics which could be interesting for other groups in the institute. Members of the team accomplished some remarkable achievements during the evaluated period. Two illustrations are

1 Computational Methods
2 Theoretical Computer Science
3 Nonlinear Modelling
4 Medical Informatics and Biostatistics
5 Nonlinear Dynamics and Complex Systems
6 Optimization and Systems
7 Fundamental Topics

[5] **M. Fiedler**: *Matrices and Graphs in Geometry*. Cambridge University Press, Cambridge, 2011,

[6] **V. Kůrková**: Complexity estimates based on integral transforms induced by computational units. *Neural Networks.* 33:160–167, 2012.

The book [5] is without doubts one of the strongest achievements of the institute in the evaluation period. Its author, professor Miroslav Fiedler, a mathematician of worldwide prestige, has been for many years one of the scientific pillars of the institute.

Notable result [6] of Věra Kůrková from 2012 reduces complicated mathematical assumptions about properties of a class of neural network elements to very natural assumptions and proves rate of approximation. It turns out that geometrical properties of input data are important. For example for data in d-dimensional sphere the fast convergence is guaranteed, whereas for d-dimensional cube not.

Team 2 focuses its attention on mathematical logic and computational complexity. In both areas it emphasises non-classical approaches and models.
During the evaluated period a considerable editorial initiative realized in the first mentioned area is the two-volume Handbook of Mathematical Fuzzy Logic, lucidly summarising state-of-the-art of the discipline. Members of the team were the editors of the handbook and substantially contributed to its content.

1 Computational Methods
2 Theoretical Computer Science
3 Nonlinear Modelling
4 Medical Informatics and Biostatistics
5 Nonlinear Dynamics and Complex Systems
6 Optimization and Systems
7 Fundamental Topics

[7] **P. Cintula**, **P. Hájek C. Noguera** (editors): *Handbook of Mathematical Fuzzy Logic* (volume 1 and 2). College Publications, London, 2011.

Mathematical Fuzzy Logic which originated and was developed in the group (particulary to the merit of professor emeritus Petr Hájek) is a synthesis of several important schools of thought of the 20th century, e. g. multivalued logics or the theory of fuzzy sets. It provides a simple apparatus for dealing with these theories, methodologically comparable with classical logic. During the evaluated period, the team members accomplished a significant thematic shift and extended their scope of interest to substructural logics.

An example of an achievement in this direction is the paper

[8] **R. Horčík**, K. Terui. Disjunction property and complexity of substructural logics. *Theoretical Computer Science* 412:3992–4006, 2011,

which at the same time illustrates an overlap with the second main area of interest of team members.

An example of an achievement within the second main area is

[9] **J. Šíma**,**S. Žák**. Almost k-wise independent sets establish hitting sets for width-3 1-branching programs. In A. Kulikov and N. Vereshchagin, editors, *Computer Science - Theory and Applications*, volume 6651 of Lecture Notes in Computer Science, pages 120–133. Springer, Berlin, 2011. (Full version is available at http://www2.cs.cas.cz/~sima/hitt1bp3.pdf),

dedicated to investigation of an important open problem in computational complexity, with the aid of branching programs - a model getting a long-term attention in the group.

Team 6 was constituted in July 2013 from several small groups and individuals coming from three different departments in the previous organizational setting. Today it aspires to interconnect several scientific streams in the institute.
The aspiration has sound backgrounds:

1 Computational Methods
2 Theoretical Computer Science
3 Nonlinear Modelling
4 Medical Informatics and Biostatistics
5 Nonlinear Dynamics and Complex Systems
6 Optimization and Systems
7 Fundamental Topics

- Stefan Ratschan (an Austrian with 12 years of experience at several foreign institutes), who leads the team, has been proficient in disciplines nurtured in different otherwise mutually non-communicating units of the institute. His scientific interest in hybrid dynamical systems (partially discrete, partially continuous) reflects the fact.
- The search for synergies among different constituents of the team (e.g. Ladislav Lukšan – a seasoned expert in optimization – and his group, Tomáš Bureš - an expert in software architecture for cyber-physical systems, or Roman Neruda interested in genetic algorithms and metalearning) has led to better mutual

understanding. This is witnessed by the report submitted by Team 6 to this evaluation exercise.

- The attention paid to team members is bringing its fruits – the professional development of Peter Franek in the past few years (bearing [10] quoted below as its fruit) can serve as an example.

Achievements of the team can be illustrated by

[10] **P. Franek**, M. Krčál: Robust satisfiability of systems of equations. In *SODA14: Proceedings of the Twenty-Fifth Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 193–203. SIAM, 2014. (Full version to appear in Journal of the ACM)

[11] **S. Ratschan**: Safety verification of non-linear hybrid systems is quasi-decidable. *Formal Methods in System Design* 44:71–90, 2014.

1 Computational Methods
2 Theoretical Computer Science
3 Nonlinear Modelling
4 Medical Informatics and Biostatistics
5 Nonlinear Dynamics and Complex Systems
6 Optimization and Systems
7 Fundamental Topics

The subject of interest of **Team 3** is environmental informatics. The team is unique in the institute in its capability to solve practical tasks requiring know-how from different disciplines. The size of the team does not allow for narrow specialization, its members have to keep a distinct flexibility and skill level in mathematics, geoscience and computer science, including high performance computing.

The team works on problems in atmospheric modelling, energy consumption and production modelling, and in traffic flow modelling. It exploits synergy ensuing from the interconnectednes of the different models employed. Its members combine solution of practical problems with basic research. Here are examples of results from the area of energy meteorology:

[12] **M. Brabec,** M. Paulescu, V. Badescu: Generalized additive models for nowcasting cloud shading. *Solar Energy* 101:272–282, 2014,

[13] **P. Juruš**, **K. Eben**, **J. Resler**, **P. Krč**, **I. Kasanický**, **E. Pelikán**, **M. Brabec**, **J. Hošek**: Estimating climatological variability of solar energy production. *Solar Energy* 98:255–264, 2013.

1 Computational Methods
2 Theoretical Computer Science
3 Nonlinear Modelling
4 Medical Informatics and Biostatistics
5 Nonlinear Dynamics and Complex Systems
6 Optimization and Systems
7 Fundamental Topics

Finis coronat opus – we have reserved **Team 1** for the end of the tour not only because of its continued high standards kept over a period of more than two decades, but also because the group has stayed on a steady thought-out course over a long-time period. Its course will serve us in Section 4 as a springboard for a prospect applicable to the whole institute.

The main research area of Team 1 is matrix computations, including direct solvers. Examples of achievements of the team in the evaluated period are:

[14] P. Jiránek, **Z. Strakoš**, M. Vohralík: A Posteriori Error Estimates Including Algebraic Error and Stopping Criteria for Iterative Solvers. *SIAM Journal on Scientific Computing* 32:1567–1590, 2010,

[15] J. Scott, **M. Tůma**: On Positive Semidefinite Modification Schemes for Incomplete Cholesky Factorization. *SIAM Journal on Scientific Computing* 3236:A609–A633, 2014.

In its present form, the team has four full-timers: Jurjen Duintjer Tebbens, Miroslav Rozložník, Petr Tichý, and Miroslav Tůma. A special place among part-timers belongs to Zdeněk Strakoš, one of the two founders of the group - he moved to Charles University at the beginning of 2010, but has been a leading member of the team.

The team has gained international recognition, as witnessed by various official as well as tacit signs.

The course followed since Zdeněk Strakoš and Miroslav Tůma laid the foundations of the group approximately 20 years ago, can perhaps be characterized by two goals which can be traced in some of their writings:

- To actively contribute to forming the concept of computational mathematics in contrast to succumbing to fads
- To search for the meaning of the concepts “computational” or ”computational mathematics” in unfolding the inner structure of a problem or a class of problems.

We shall use two diagrams borrowed from a recent publication (Josef Málek and **Zdeněk Strakoš**, Preconditioning and the Conjugate Gradient Method in the Context of Solving PDEs, SIAM Spotlights, 2015), to make (at least schematically) important observations about the sustained course of the group. We shall refer to them in Section 4.

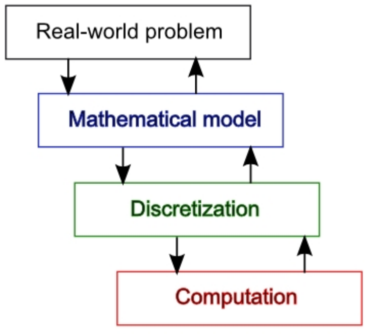


Fig. 2

Fig. 2 illustrates the frequently used sequence leading from a real-world problem to its numerical solution implemented on a computer. The research interests of Team 1 can be localised at the block ”Computation” of the diagram. However, the above mentioned long-term course of Team 1 insists that individual blocks in the diagram should not break away and create solely their own agenda, but each of them should be considered in the context of the whole sequence.

An organizational rendering of this principle was the establishment of the Nečas Center for Mathematical Modeling (NCMM) in 2013 in which the team members participate together with experts from the Charles University and the Mathematical Institute of CAS. NCMM covers the whole sequence from Fig. 2.

Fig. 3 indicates that the above mentioned principle can lead and in the case of some Team 1 members has led to a considerable paradigm shift. The conjugate gradient method (an object of long-term studies of the team, together with other Krylov sub-space methods) can be interpreted as a concept at the heart of the whole sequence from Fig. 2.

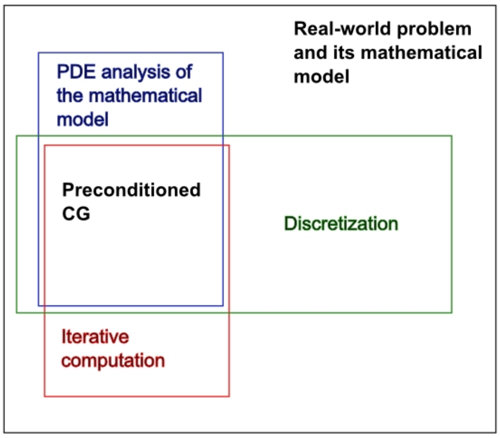


Fig. 3

Research Report of the team in the period 2010–2014

Institute	Institute of Computer Science of the Czech Academy of Sciences
Scientific team	Department of Computational Methods

The scientific activities of the current members of the Department of Computational Methods in the period 2010-2014 concern primarily matrix computations. In this field of basic research combining computer science and mathematics, the department's results comply with high international standards. The main characteristics of the department between 2010 and 2014 will be described in the following way:

1. Brief introduction into the research area of the department
2. The structure of the department
3. Main scientific results in the period 2010-2014
4. Significant conference activities

5. Other international activities and recognition

6. Pedagogical activities, other activities and recognition on the national level

1. Brief introduction into the research area of the department

The numerical solution of many real-world problems from science and engineering can be understood as a sequence of sub-problems, i.e., a *process involving several levels*. The given problem can often be first formulated (modeled) as a continuous mathematical problem, e.g., a partial differential equation. The mathematical problem must next be discretized to define an approximation of the solution in a finite dimensional space, which leads to an algebraic problem with a finite number of unknowns. The last level of the process is usually the solution of a problem from numerical linear algebra or optimization, which is implemented on a computer using finite precision arithmetic. During the *subsequent approximations* of the original problem, certain errors are made. For the efficient solution of the original problem, it is crucial to *understand these errors* and their interactions. If on one level some approximation error arises, it is pointless to solve problems of a lower level exactly; it suffices to find a sufficiently good approximation of their solutions.

Among a wide range of topics from computational mathematics, issues concerning matrix computations (numerical linear algebra) form the main focus of the department. It specializes in the development, analysis and implementation of *iterative methods* and *sparse direct solvers* for solving systems of linear algebraic equations, their preconditioning, least squares problems and to a lesser extent, eigenvalue problems. The goal thereby is to regard iterative methods as part of the above process, into which they must be integrated efficiently. This requires a thorough theoretical understanding of these methods (questions of convergence, error estimates), and the need to analyze their behavior in finite precision arithmetic when implemented on a computer. The team's long-term research efforts are consistently devoted to these questions.

The results of the department can be divided into *theoretical work* treating mathematical aspects of the considered methods, results on the *numerical stability of algorithms*, which give users important information about the reliability of calculations, the design of *new algorithms and implementations* leading to more efficient solution procedures, and finally *applications* to solve specific real-world problems. The team has achieved significant results in particular for iterative methods that seek solutions in so-called Krylov subspaces (Krylov subspace methods). This is an important class of iterative methods, especially suitable for solving systems with very large, sparse matrices. A monograph focusing on these methods and including a number of results of the team is *Krylov subspace methods – Principles and Analysis*, by J. Liesen and team member Z. Strakoš (Oxford University Press, 2013).

2. The structure of the department

The current members of the department consist of three leading scientists (Z. Strakoš, M. Tůma and M. Rozložník), five other research fellows, two postdocs and two PhD. students:

Research fellows: Prof. Z. Strakoš (age 58), Prof. M. Tůma (56), Assoc. Prof. M. Rozložník (46), Dr. J. Duintjer Tebbens (42), Dr. P. Tichý (42), Dr. Z. Tošner (39), Dr. I. Hnětynková (35) and Dr. M. Plešinger (35).

Postdocs: Dr. M. Lanzendörfer (35) and Dr. K. Morikuni (30).

Doctoral students: J. Papež (28) and M. Kubínová (28).

In the beginning of the nineteen nineties, Z. Strakoš started to build, together with M. Tůma and M. Rozložník, a research group that grew out to a well-established school, solving several open problems and earning international awards such as the SIAM Activity Group on Linear Algebra Prize (Z. Strakoš, in 1994, jointly with A. Greenbaum) and the SIAM Outstanding Paper Prize (M. Tůma, in 2001, jointly with M. Benzi). By 2010 the department contained, besides the matrix computations team, several subgroups specialized in closely related area's: Nonlinear optimization and programming (leading personality: Prof. L. Lukšan), interval arithmetic and verification (main personalities: Prof. J. Rohn and Dr. S. Ratschan) and matrix theory (prof. M. Fiedler). The reorganization of the structure of the Institute in 2013 reduced the department essentially to the small subgroup working on matrix computations (except for M. Lanzendörfer, who works in mathematical modeling and Z. Tošner who joined the team later in the context of using iterative methods to solve nuclear magnetic resonance problems). Most members have teaching and other pedagogical duties at universities across the country. Members whose principal engagement is elsewhere (not at the Institute) are M. Lanzendörfer, M. Plešinger, I. Hnětynková, Z. Tošner and Z. Strakoš. M. Rozložník was head of department from 2010 until 2013 and P. Tichý from 2013 to 2014. Since October 2014, the department is lead by the director of the Institute. More detailed information about the research fellows of the department can be found on their personal webpages.

3. Main scientific results in the period 2010-2014

The main scientific results were published in international journals such as the journals of the Society of Industrial and Applied Mathematics (SIAM) or the Association for Computing Machinery (ACM). We will use the abbreviations SISC for SIAM's Journal on Scientific Computing and SIMAX for SIAM's Journal on Matrix Analysis and Applications.

The first year of this period saw the publication of a major work on the interplay between approximation errors on the level of discretization and the matrix computations level. The paper *A Posteriori Error Estimates Including Algebraic Error and Stopping Criteria for Iterative Solvers* in SISC by P. Jiránek, Z. Strakoš and M. Vohralík presents a rigorous mathematic treatment of the inclusion of numerical linear algebra errors in a posteriori error estimates when solving partial differential equations. This leads to efficient stopping criteria for the iterative methods on the matrix computations level, thus saving potentially orders of magnitude of computational costs. The numerical behavior of several orthogonalization schemes in relation to preconditioning were the main topic of *Numerical Stability Of Orthogonalization Methods With A Non-Standard Inner Product*, by M. Rozložník, M. Tůma, A. Smoktunowicz and J. Kopal. (BIT Numerical Mathematics 2012).

Several publications introduced new algorithms. The paper *On Efficient Numerical Approximation of the Bilinear Form* $c^*A^{-1}b$ (Z. Strakoš and P. Tichý, SISC 2011) presents a method of choice for the given problem, including a justification for its use, a numerical stability analysis and links with the field of matching moments, which enable to generalize the underlying theory to the non-Hermitian case. *On Positive Semidefinite Modification Schemes For Incomplete Cholesky Factorization* (J. Scott and M. Tůma, SISC 2014) introduces a robust limited memory method, now available in the top level HSL software library, for incomplete factorization. Incomplete factorization is widely used to precondition (accelerate) Krylov subspace methods for solving linear systems. The main idea is to drop small entries during the factorization process. In *On Incremental Condition Estimators In The 2-Norm* (J.

Duintjer Tebbens and M. Tůma, SIMAX 2014) a way to estimate with enhanced accuracy the 2-norm condition numbers of submatrices in the factorization process is derived, possibly leading to more robust dropping rules. *Partitioned Triangular Tridiagonalization* by M. Rozložník, G. Shklarski and S. Toledo (in ACM Transactions on Mathematical Software, 2011) describes a new method to bring symmetric matrices to so-called tridiagonal form. Numerical stability is studied and experiments show that the method is competitive with state-of-the-art solvers implemented in LAPACK.

Theoretical work included new results on the convergence behavior of the GMRES method, a standard Krylov subspace method for nonsymmetric linear systems (*Properties of Worst-Case GMRES* by V. Faber, J. Liesen and P. Tichý, SIMAX 2013; *Any Ritz Value Behavior Is Possible for Arnoldi and for GMRES* by J. Duintjer Tebbens and G. Meurant, SIMAX 2012). The paper *The Core Problem within a Linear Approximation Problem AX≈B with Multiple Right-Hand Sides* (I. Hnětynková, M. Plešinger and Z. Strakoš, SIMAX 2013) is also of theoretical nature. The core problem approach is an efficient way to solve total-least-squares problems, a generalization of least-squares problems. The topic of the paper is the highly non-trivial situation arising with multiple right-hand sides. It presents a rigorous mathematical background for computations in this situation. The solution of ordinary least-squares problems with a preconditioned iterative method was considered in *Preconditioned Iterative Methods for Solving Weighted Linear Least Squares Problems* (R. Bru, J. Marín, J. Mas and M. Tůma, SISC 2014). Several algorithmic improvements lead to an enhanced robustness of the method.

4. Significant conference activities

Perhaps the most prominent conference in the field of matrix computations is the triannual Householder symposium. It is named after one of the founders of the field, who started the conference in the early sixties in the USA (for the history of the conference, see https://sites.uclouvain.be/HHXIX/History.html). Until today, participation is on invitation only. Since the nineteen nineties, members of the team have regularly been invited, in particular Z. Strakoš gave several plenary talks at the symposium. In the period 2010 - 2014, seven members of the department were invited to the XVIIIth symposium (June 2011, Lake Tahoe, https://sites.google.com/a/lbl.gov/hh11/home) and to the XIXth symposium (June 2014, Spa, http://sites.uclouvain.be/HHXIX/), which is a remarkably strong representation for a single research group. In 2011, P. Tichý gave a plenary lecture and J. Duintjer Tebbens won the (shared) best poster prize.

Z. Strakoš was member of the Scientific Committee of the Householder symposium from 2005 to 2014 and is member of the ICIAM 2015 Scientific Program Committee from 2013 to 2015.

A selection of plenary lectures and invited participations of the team members at international conferences is**:**

2010: Plenary talk at the *Ninth China Matrix Theory and Applications International Conference* (http://math.shu.edu.cn/CLAS2010/English/) in Shanghai, July (M. Tůma), plenary talk at the *16th International Linear Algebra Society Meeting* (http://www.dm.unipi.it/~ilas2010/) in Pisa, June (Z. Strakoš).

2011: Plenary talk at the XVIIIth Householder symposium (P. Tichý), invited talk at the XVIIIth Householder symposium (J. Duintjer Tebbens, I. Hnětynková, M. Plešinger, M. Rozložník, Z. Strakoš, M. Tůma), minisymposium invitation at the *ICIAM* conference (http://www.iciam2011.com/) in Vancouver, July (P. Tichý), minisymposium invitation at the *SIAM Optimization* conference (http://www.siam.org/meetings/op11/) in Darmstadt, May (J. Duintjer Tebbens).

2012: Plenary talk at the *4th International Conference on Numerical Algebra and Scientific Computing* (http://lsec.cc.ac.cn/~NASCNAG/NASC_pages/Conf_pages/NASC12_pages/) in Dalian, October (M. Rozložník), plenary talk at the *BIRS Workshop Model reduction in continuum thermodynamics: Modeling, analysis and computation* (http://www.birs.ca/events/2012/5-day-workshops/12w5029) in Banff, September (Z. Strakoš), invited talk at the international conference *Structured Matrix Computations in Non-Euclidean Geometries: Algorithms and Applications* (http://www-lmpa.univ-littoral.fr/SMC-NEGAA2012/) in Luminy, October (M. Rozložník), minisymposium invitation at the *SIAM Conference on Applied Linear Algebra* (http://www.siam.org/meetings/la12/index.html) in Valencia, June (Z. Strakoš).

2013: Plenary talk at *Domain Decomposition Methods for Optimization with PDE Constraints* (http://www.unige.ch/math/ascona2013/) in Ascona, September (Z. Strakoš), plenary talk at *Preconditioning of Iterative Methods - Theory and Applications* (http://pim13.fsv.cvut.cz/) in Prague, July (Z. Strakoš), minisymposium invitation at the *25th Biennial Numerical Analysis Conference* (http://www.nais.org.uk/events-forums/25th-biennial-numerical-analysis-conference) in Glasgow, June (J. Duintjer Tebbens), invited talk at *EQUADIFF 2013* (http://equadiff.zcu.cz/) in Prague, August (Z. Strakoš), minisymposium invitation at *ENUMATH 2013* (http://enumath2013.epfl.ch/) in Lausanne, August (Z. Strakoš).

2014: Invited talk at *Snapshots of Numerical Analysis* (http://anchp.epfl.ch/mhg70) in Lausanne, October (M. Rozložník), invited talk at the XIXth Householder symposium (J. Duintjer Tebbens, I. Hnětynková, M. Plešinger, M. Rozložník, Z. Strakoš, P. Tichý, M. Tůma).

The results of the team were also presented at numerous other presentations (on average ca. 50 per year), for example as contributed talks on international conferences, at international workshops and during visits of the individual members to research institutes abroad.

The department organized or co-organized the following international workshops (50 to 100 participants): The GAMM Linear Algebra Activity Group meeting in 2012 (http://www.cs.cas.cz/gamm/), the MORE workshop on Implicitly constituted materials: Modeling, analysis, and computing in 2013 (http://www.cs.cas.cz/more2013/) and the MORE workshop on Modeling, analysis and computing in nonlinear PDEs (http://www.cs.cas.cz/more2014/). Besides that, small-scale international workshops were co-organized (AIME series, see http://homepages.laas.fr/henrion/aime@cz15/ for links to the history of the series in the period 2010-2014).

5. Other international activities and recognition

All team members collaborate intensively with research groups abroad. Examples of long-term collaboration, often resulting in series of papers, are the results obtained with J. Scott from Oxford's STFC national laboratory (M. Tůma), with J. Liesen from the TU Berlin (Z. Strakoš and P. Tichý), with G. Meurant from Paris (J. Duintjer Tebbens, Z. Strakoš and P.

Tichý) or R. Bru from Valencia Polytechnical University (M. Tůma). The team obtained national grants specifically for collaboration with these and other groups (principal investigator: M. Tůma).

Some team members were between 2010 and 2014 involved in peer-review of international grant applications. Z. Strakoš served, from 2008, on the ERC Advanced Grants Evaluation Panel for Computer Science and Information and was named its chair in 2014 (http://erc.europa.eu/sites/default/files/document/file/Panel_Chairs_AdG_2014.pdf), I. Hnětynková was referee for Horizon grant applications in 2014, P. Tichý for german DFG Sonderbereich and belgian KU Leuven applications.

In the period 2010 until 2014, most members of the younger generation completed (or started) a stay abroad (M. Plešinger at ETH in Zürich (11 months), J. Papež at Université Pierre et Marie Curie in Paris (3 months), M. Kubínová at Emory University in Atlanta (started in September 2014).
K. Morikuni was awarded the SIAM student paper prize in 2013 (before he joined the department).

A clear sign of international recognition is the fact that Strakoš was selected *SIAM fellow* for advances in numerical linear algebra, especially iterative methods, in 2014. I. Hnětynková was awarded the international Visegrad Group Academies Young Researcher Award for young researchers in Applied Mathematics in 2014.

6. Pedagogical activities, other activities and recognition on the national level.

Information about most activities on the national level, including pedagogical activities, are communicated in a separate form. In this section only information not available on the form is mentioned.

The department regularly organizes a winter school (mostly in Czech), the Seminar of Numerical Analysis, with tutorial lectures for the Czech public. In the period 2010-2014, three winter schools were organized by the department (in 2010, 2012 and 2014, http://www.cs.cas.cz/sna10/indexe.htm, https://kmd.fp.tul.cz/old/SNA/sna12.htm, http://www.cs.cas.cz/sna2014/). The department also organizes the seminar of computational methods at the Institute, which hosted, between 2010 and 2014, about 30 foreign guest speakers (http://www2.cs.cas.cz/semincm/).

The Bernard Bolzano medal of the Academy of Sciences of the Czech Republic for Merits in Mathematical Sciences was awarded to Z. Strakoš in 2013. Until 2013, M. Tůma was deputy head of the Academy of Sciences of the Czech Republic. The Jaroslav Jirsa price for the best textbook of Charles University in 2012 in the natural sciences was assigned to: J. Duintjer Tebbens, I. Hnětynková, M. Plešinger, Z. Strakoš and P. Tichý: *Analýza metod pro maticové výpočty - Základní metody.* M. Kubínová was granted a Fullbright stipendium. The second price in the Babuška competition for the best diploma thesis in computational mathematics was awarded to J. Papež. The team was successful with grant applications at the Czech Science foundation and at the program for internal support of projects of international collaboration of the Academy of Sciences of the Czech Republic.

In 2013 the Nečas Center for Mathematical Modeling was cofounded by the Institute (together with the Faculty of Mathematics and Physics, Charles University and the Institute of Mathematics of the Academy of Sciences of the Czech Republic). The center is a research platform to coordinate and promote research and education activities of several Czech Republic based research teams working in theoretical and applied mathematics. The philosophy of the center is based on a close interaction of researchers from diverse fields, see http://ncmm.karlin.mff.cuni.cz/ for a detailed description. The team members M. Rozložník and Z. Strakoš belong to the executive board of the center. The MORE workshops mentioned earlier were organized within the activities of the center.

Collaboration in solving problems of real-world applications took place among others with the Institute of Physics of the Academy of Sciences of the Czech Republic (M. Rozložník, M. Tůma), in the field of nuclear magnetic resonance problems (Z. Tošner), with the Mathematical Institute of Charles University concerning flow and (in)compressible fluids problems (M. Lanzendoerfer) and with the Faculty of Pharmacy of Charles University in statistical problems (J. Duintjer Tebbens).

Institute	Institute of Computer Science of the Czech Academy of Sciences

Scientific team	Department of Theoretical Computer Science

Objectives and research areas

Research in the *Department of Theoretical Computer Science* focuses on logic and computation, a coherent research area central to theoretical computer science, but indispensable also in applications. The researchers in the Department seek to gain a deeper understanding of the processes of reasoning and computation, employing a wide range of methods and approaches. A broad aim of this kind naturally leads to the investigation of a wide range of both foundational and specialized issues in mathematics and theoretical computer science. An important common trait of our work is frontier research: we strive to broaden the repertoire of approaches that are considered standard in our respective areas.

This concerns now well established areas of logic, such as substructural, fuzzy and modal logics, while in theoretical computer science we investigate fundamental problems in the theory of computation but also venture into areas dealing with specialized non-standard computational models, such as neural nets and branching programs.

Logic and computation share a lot of unifying themes. For instance, department members have investigated computational complexity of various decision problems in logic and seek to find general properties that determine algorithmic behavior of logics. The research areas investigated during the assessment period by members of the Department are depicted in Figure 2.

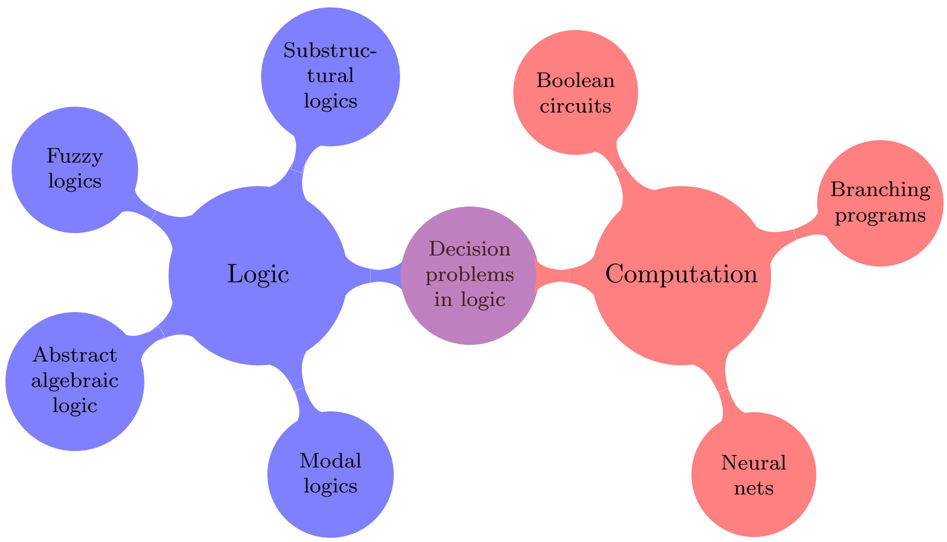


Figure 2: The research areas investigated during the assessment period by the Department.

Team structure

As shown in Figure 1, the Department is well balanced in terms of age, career stage and research experience. This, and the ability of the team to venture into new research topics, ensures viability for the future. The team had 19 members by the end of 2014. Excepting an emeritus member (Petr Hájek), Figure 3 shows the team structure, expressed as full time equivalent (FTE), in particular qualification categories. The total FTE of the team at the end of 2014 was 12.4. It is worth mentioning that the Institute of Computer Science underwent a major structural change in mid 2013, increasing the number of its departments from 4 to 7. Some previous members of the Department had moved to other (new) departments. The current team is therefore smaller and more compact than in 2010.

During the evaluated period, the Department employed 1 foreign scientist (Carles Noguera), 3 foreign postdocs (José Gil-Ferez, Félix Bou, and Tomoyuki Suzuki) and 1 foreign PhD student (Paolo Baldi).

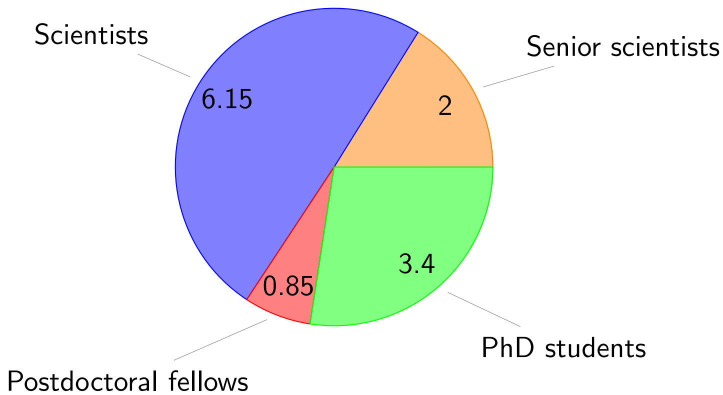


Figure 3: The team structure according to FTE in particular qualification categories.

Research highlights

Research highlights in the Department of Theoretical Computer Science range from important results answering specific questions to carrying out comprehensive research programmes. Below is a selection of examples from the above-mentioned research areas.

- One of the main achievements in the research in logic is the *Handbook of Mathematical Fuzzy Logic*, prepared and published during the evaluated period [2, 3]. This two-volume compendium comprises 11 chapters, out of which 5 were written by the team members. The Handbook covers the majority of mature areas of mathematical fuzzy logic and gives an up-to-date overview of the available material in those areas; it also contains new results. Its editors, Petr Cintula, Petr Hájek and Carles Noguera, were members of the Department during the evaluated period.

- Jiří Šíma and Stanislav Žák contributed to one of the central issues in the theory of computation, namely the $\mathsf{RL} = \mathsf{L}$ problem of derandomizing poly-time log-space computations. The world's best results attacking this issue are based on constructing the hitting sets for severely restricted read-once branching programs. They have achieved the construction for general read-once programs of width 3, which is cited as a breakthrough that has not been surpassed yet [5].

- Jointly with Kazushige Terui (RIMS, Kyoto University), Rostislav Horčík proved that every consistent substructural logic enjoying the disjunction property has to be necessarily PSPACE-hard [4]. This result simplifies substantially proofs of complexity lower bounds and surpasses commonly used proof-theoretical methods, which are applicable only in particular cases. Another success within the area of decision problems in logic, due to Karel Chvalovský and Rostislav Horčík, is a solution of an almost 20 years old problem from proof theory concerning decidability of intuitionistic logic without the rules of weakening and exchange. This result [1] was accepted to Journal of Symbolic Logic at the end of 2014.

Research output

A summary of publications of department members can be found in Table 1. The contribution of team members to the above publications/results is almost always proportional to the number of authors from our team. As usual in theoretical computer science and mathematics, authors are listed in the alphabetical order and authorship distributes uniformly among authors and is based on a significant contribution to the content of the work.

	2010–2014	**2015$^+$**
Impacted journal articles	39	10
Other journal articles	4	0
Books	3	0
Book chapters	11	4
Conference papers	45	0
Software	2	0
Total output	104	14

Table 1: Research output of the Department during 2010–2014 and outputs accepted for publication or published after the evaluation period.

Although department members focus mainly on theoretical research, one of the members (Petr Savický) has contributed to the development of open-source statistical software R with millions of users via authorship of new extension packages and providing patches to the core system. For details see the following websites:

- `http://www.r-project.org/contributors.html`
- `http://cran.at.r-project.org/web/packages/CORElearn/`
- `http://cran.at.r-project.org/web/packages/rngSetSeed/`

Funding

The Department has been successful in attracting external funding (see Appendix 3.1, grants no. 7–26). During the years 2010–2014 the Institute income from the running projects whose principal investigator or co-investigator was from the Department was approximately 48 millions CZK (i.e., approx. 1.8 M€). Table 2 provides an overview of the internal and external sources of funding of the Department.

	2010	**2011**	**2012**	**2013**	**2014**	**Sum**
Internal funding via Czech Acad. of Sci.	5	3.5	4.2	3.9	3.8	20.4
External funding via research grants	10.2	9.9	8.4	6	6.6	41.1
Total	15.2	13.4	12.6	9.9	10.4	61.5

Table 2: Sources of research funding in millions of CZK (not containing overheads).

Quality and scientific relevance

In the following, some facts showing the impact of the research of department members on the scientific community are collected. According to *Web of Science* (WOS), the team members' works have more than 2800 citations (approx. 2200 without self-citations), out of which 1200 were received during 2010–2014. The collective h-index of the team, according to WOS, is 27. Besides the above-mentioned numbers of citations, the department members are delighted that their results are utilized by internationally established researchers. For instance, one of our main achievements [5] was used and cited by Parikshit Gopalan (Microsoft Research) during his lecture at *Institute of Advance Study, Princeton* (`https://video.ias.edu/csdm/gopalan`). Another example is a blog post by Richard J. Lipton (`https://rjlipton.wordpress.com/2013/09/12/teacher-teach-yourself/`) explaining his teaching experience of a classic theorem from computational complexity due to our team member Stanislav Žák.

The department members gave the following invited lectures at international conferences and workshops.

- R. Horčík. *Residuated Lattices, Regular Languages, and Burnside Problem.* Topology, Algebra, and Categories in Logic, Nashville, USA, 2013.

  `http://www.math.vanderbilt.edu/~tacl2013/`

- R. Horčík. *Quasi-equational Theory of Square-increasing Residuated Lattices is Undecidable.* Logic, Algebra and Truth Degrees, Kanazawa, Japan, 2012.

  `http://www.jaist.ac.jp/rcis/latd12/`

- P. Cintula. *First-order non-classical logics: an order-based approach.* Compositional Meaning in Logic, Vienna, Austria, 2014.

  `http://sqig.math.ist.utl.pt/GeTFun/2.0/`

- O. Majer. *Semantic Games for Łukasiewicz Logic.* Workshop Logic and Games, Vienna Summer of Logic, Austria, 2014.

  `http://www.logic.at/logic-and-games-2014/`

- Z. Haniková. *Set theory in many-valued logics.* Post-graduate workshop on alternative set theories, Amsterdam, Netherlands, 2013.

  `http://www.math.uni-hamburg.de/home/loewe/AST2013/`

- P. Cintula. *Mathematical Fuzzy Logic: First-Order and Beyond.* International Workshop Information, Uncertainty, and Imprecision, two lectures tutorial, Olomouc, Czech Republic, 2013.

  `http://mcin.upol.cz/SSWIU-2013/`

During the evaluated period, the department members had 21 foreign coauthors coming from 10 countries. Among the home institutes of our coauthors are for example *Research Institute of Mathematical Sciences, Kyoto University; University of Denver; University of Bern; University of Melbourne; Vienna University of Technology; University of Leicester; Johannes Kepler Universität Linz.* The Department also hosted 13 foreign guests coming from 9 countries.

References

[1] Karel Chvalovský and Rostislav Horčík. Full lambek calculus with contraction is undecidable. To appear in *Journal of Symbolic Logic*.

[2] Petr Cintula, Petr Hájek, and Carles Noguera, editors. *Handbook of Mathematical Fuzzy Logic. Volume 1*, volume 37 of *Mathematical logic and foundations*. College Publications, 2011.

[3] Petr Cintula, Petr Hájek, and Carles Noguera, editors. *Handbook of Mathematical Fuzzy Logic. Volume 2*, volume 38 of *Mathematical logic and foundations*. College Publications, 2011.

[4] Rostislav Horčík and Kazushige Terui. Disjunction property and complexity of substructural logics. *Theoretical Computer Science*, 412(31):3992–4006, 2011.

[5] Jiří Šíma and Stanislav Žák. Almost k-wise independent sets establish hitting sets for width-3 1-branching programs. In A. Kulikov and N. Vereshchagin, editors, *Computer Science - Theory and Applications*, volume 6651 of *Lecture Notes in Computer Science*, pages 120–133. Springer, Berlin, 2011. Full version available at `http://www.cs.cas.cz/~sima/hitt1bp3.pdf`.

Research Report of the team in the period 2010–2014

Institute	Institute of Computer Science of the Czech Academy of Sciences

Scientific team	Department of Nonlinear Modelling

Area of research

The team of nonlinear modelling works in the area of *environmental informatics,* which can be characterized as an interdisciplinary field concerned with the questions tightly connected to environmental and related topics. This field has been changing dramatically in recent years, particularly thanks to the boom of available data which come from both conventional observations and by exploitation of non-traditional measurements, such as sensor networks, cell phones, floating car data, satellite data in general and GPS data in particular. This change, as well as the advancements in technologies in other fields, brings number of new problems and challenges. An interconnection of various approaches, which include methods of mathematical modelling, mathematical statistics, high performance computing, and machine learning is often the best way to tackle the environmental problems of modern society.

Our team is specifically oriented towards the atmospheric modelling, modelling of energy consumption and production, and traffic flow modelling. These fields are inter-related and there exists a number of synergies when solving the specific problems. Examples where the team know-how can be leveraged are questions involving air-quality and emission modelling, where all the fields of atmospheric modelling, energy, and transportation are tightly connected. Some of the results of our team go even further – e.g. in the assessment of the impact of air quality on human health. Another example of the connection is the field of energy meteorology, where our team has been active in the past years and where the team experience in atmospheric modelling and energy modelling is advantageous, e.g., for the renewable power sources modelling.

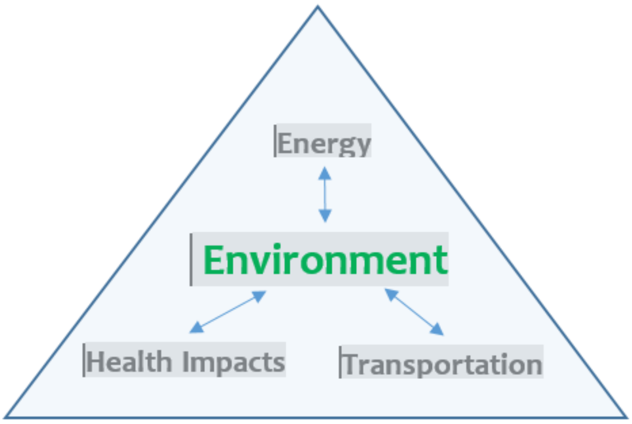


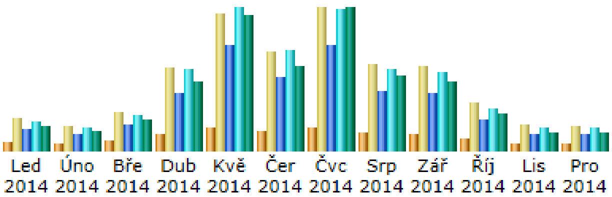
Figure 1 The main application areas of our research and their interconnections

The tools used for our research are important especially for the applied research which involves modelling real-world cases and processing large volumes of often noisy real-life data. Various Eulerian chemical transport models and numerical weather prediction models are used within our group, as well as variety of both general purpose and specialized mathematical software. Lots of other software utilities for pre- and post-processing, model coupling, visualization and data processing have been developed in-house and the whole computational system has to be often run and maintained in parallel regime on HPC (high-performance computing) clusters.

This workflow involving a mix of theoretical research, data handling, modelling and HPC requires cooperation of the team members. The tight teamwork makes possible to handle real-life problems. The size and tight integration of the team is therefore a fairly important factor, since we are big enough to solve applied problems with “big data” on one hand and small enough to understand each other’s work and come with original solutions to new problems on the other hand. We therefore complement the teams which are either smaller – doing mostly theoretical research often using idealized computer models and cases – on one side and the large centres which are often specifically focussed on the operational aspects of, e.g., weather forecasts, on the other side.

Before stating strictly scientific results let us mention two activities which are important for the team and lead to a number of scientific challenges connected to recent technological and societal developments. They illustrate well the work of the team and the background upon which the scientific research is conducted.

The first specific activity is the project Medard [1] which is our team's attempt to bring the forecasts of weather and air quality for the Czech Republic to the public. The forecasts are computed operationally - every six hours a new forecast for the 3 days ahead is computed. This system is online for the past 10 years and especially in the first years it was the only numerical weather and air quality prediction in the form of maps publicly available for the Czech Republic. Since that time, many developments, particularly in chemical transport modelling, have been adapted by official national modelling system thanks to the collaboration of our team with the Czech Hydrometeorological Institute. Our forecasts enjoyed sustained high popularity during the period 2010-2014. Figure 2 shows that the web with our weather predictions has accumulated 100-750 thousands of visits monthly in 2014, depending on the season.



Měsíc	Unikátní návštěvy	Počet návštěv	Stránek	Hity	Bajtů
Led 2014	44869	168195	7887035	11091801	116.42 GB
Úno 2014	38228	131646	6012537	8463876	91.36 GB
Bře 2014	54468	205478	9684791	13705894	144.78 GB
Dub 2014	88495	434822	22006240	30547904	327.42 GB
Kvě 2014	123977	718751	39904091	53861857	648.63 GB
Čer 2014	102365	520495	27916079	38003236	406.06 GB
Čvc 2014	122881	748591	39520979	53801805	683.96 GB
Srp 2014	93283	449484	22493479	30776783	358.47 GB
Zář 2014	89698	446774	21665982	29807653	330.62 GB
Říj 2014	61715	251541	11771173	16061952	176.33 GB
Lis 2014	40671	137869	6116756	8452530	91.05 GB
Pro 2014	36288	129836	6184522	8414974	89.80 GB
Celkem	896938	4343482	221163664	302990265	3464.91 GB

Figure 2 Screenshot of the Medard web statistics for the year 2014. The number of visits is in the third (yellow) column. Each line represents one month of the year 2014. The statistics are generated using AWStats utility.

Having operational weather and air quality forecast with popular web presentation is not only creating a great way for the outreach to general public but it also constitutes a focal point to a large part of our research work. Having hands-on experience with everyday's problems of atmospheric modelling and forecasting helps us to build skillset useful for solving the problems in the fields such as data assimilation or energy meteorology.

Another important activity which paves the way to a number of interesting open problems is the field of energy consumption modelling. The team has long-standing experience with various aspects of energy production and consumption modelling. Established collaboration with commercial and industrial partners has led to a number of practical improvements and to the standardisation of mathematical methods. These methods are used in natural gas modelling and accounting on the national level [2, 3, 4]. This collaboration and direct contact with the data, models and approaches used in energy production and consumption modelling applications motivate scientific research in this field. The review paper from year 2012 [5] cites 7 scientific results of our team in the area of natural gas consumption forecasting.

Structure of the team

As of the end of year 2014, the team consisted of

- 2 senior researches (1 full-time, one part-time 0.15 FTE),
- 7 researchers (3 full-time, 4 part-time with total 1.3 FTE),
- 2 post-doctoral fellows (1 full-time, 1 part-time 0.5 FTE),
- 2 associate scientist (part-time 0.7 FTE),
- 1 research assistant (part-time 0.5 FTE),
- 3 graduate students (2 full-time, 1 part-time 0.8 FTE).

Two of the researchers moved up from the category of post-doctoral fellows in the years 2010-2014 and the two post-doctoral fellows defended their Ph.D. theses recently and moved up from the category of graduate students. This increases the team capacity to mentor and involve a larger number of graduate students.

The personal composition (specifically the researchers) and the scientific orientation of the team has been fairly stable throughout the various organizational changes in the Institute of Computer Science. The founder of the team is the only full-time senior researcher - Emil Pelikan, whose work includes setting the scientific agenda of the team, organizational work, project management, and junior team members mentoring. The other senior researcher is Jan Mandel who is the external team member for the duration of a grant project. Since his home institution is University of Colorado, Denver, we include only his results made in collaboration with other members of our team. A valuable contribution for the team is his involvement in mentoring team members in early-stage career.

Important results

The result list is fairly broad and touches a lot of scientific areas due to the interdisciplinary orientation of the team members. Nevertheless, there are two clusters of results which deserve specific attention and which constituted the core of activities in the period 2010-2014.

Energy meteorology is an interdisciplinary field which has gained importance in recent years due to the increasing dependence of energy production and consumption on meteorological conditions. Our team successfully combines its expertise in both weather modelling and energy modelling. The majority of our results in the years 2010 - 2014 is in the area of photovoltaic power production modelling and forecasting. The results, improving various aspects of photovoltaic power production on different temporal and spatial scales, have been published in top scientific journals in the field [6, 7, 8, 9, 10, 11]. Our team was also pleased by the successful participation in benchmarking exercise on short-term forecasting models for renewable generation, which was organized by the COST Action 1002 WIRE – Weather Intelligence for Renewable Energies. Our team has submitted the forecasts for the photovoltaic power prediction for Catania, Italy. Our results had the best (the lowest) root-mean-square error (RMSE) and the second best mean absolute error (MAE) (benchmark announcement and congratulation letter http://www.ustavinformatiky.cz/docs/WIRE_oceneni_uiavcr_2015.pdf).

Another notable group of results belongs to the field of data assimilation. Data assimilation in atmospheric modelling is the process of combining the model forecasts and available observation data to obtain the best possible estimate of the atmospheric state. It is one of the most important steps in order to have good forecasts and the process of data assimilation is the most computationally expensive part of weather prediction – especially for the global numerical weather prediction models, which are run on large-scale computer clusters. Our team focuses on the data assimilation in the chemical transport models. One of the team members, Jaroslav Resler, participates in the CMAQ adjoint core group and contributes to the development of the adjoint code of CMAQ model – an Eulerian chemical transport model preferred by a number of organizations worldwide. He has been responsible specifically for the parallelization of the code and the optimisation of the MPI (message passing interface) code for the real-world cases.

The results of our data assimilation work include inverse modelling studies, which have been extended to an estimation of emission profiles [12], and later also to an assessment of the impacts of individual emission sources on mortality [13]. Another team member, Kryštof Eben, co-authored a large review paper [14] on operational air quality modelling in Europe, where he has been responsible for the part about data assimilation. Theoretical aspects of data assimilation are currently being investigated – see [15] which has been submitted to Nonlinear Processes in Geophysics.

Projects

Projects are the main driving force of the team's research. They provide the platform for the collaboration, for the formulation of the goals and for day-to-day team operation. The proportion of institutional and external funding for the team has been consistently around 50/50% in the years 2010-2014.

The portfolio of the past and present projects follows the research agenda of the team. The public funding comes from diverse sources which improves the robustness since the team manifests the ability to obtain funding from different bodies and programmes and does not depend on single source of external funding in changing landscape of the science funding structure. On the other hand, this diverse project portfolio means that team members must expect higher complexity and effort when both writing project proposals and administrating running projects, since each funding source has different rules and different priorities.

The major projects funded from public resources in the period 2010-2014 were:

- LD12009 *Advanced methods for energy production forecasting by photovoltaic systems using high resolution NWP models* – funded by Ministry of Education,
- TA02031411 *Increasing the usage of parking capacity on highways using prediction models* – funded by Technology Agency of the Czech Republic,
- M100300904 *Greenhouse gases emission reduction using information technologies* – funded by the Czech Academy of Sciences,
- SP/1A4/107/07 *Improvement and specification of modelling of air pollution and acquisition of fundaments for prediction of health effects* – funded by Ministry of Environment.

Ongoing projects which have started in the period 2010-2014 are:

- GA13-34856S *Advanced random field methods in data assimilation for short-term weather prediction* – funded by the Grant Agency of the Czech Republic,
- RIGTC/2014/DARTMA/245 *Development and Assessment of Regional Tropospheric Model for Augmented GNSS Positioning and Navigation Development* – as a subcontractor, funded by European Space Agency.

The team also regularly participates in the projects of EU COST programme which do not provide the funding for research but only for networking. They are nevertheless a great platform for meeting other teams working in the same research area and for building collaborations across the scientific community. A large part of the research in the period 2010-2014 in the field of energy meteorology has been conducted with the aid of COST Action ES1002 WIRE: *Weather Intelligence for Renewable Energies* which has concluded in 2014. An ongoing project which focuses on GNSS meteorology is COST Action ES1206 GNSS4SWEC: *Advanced Global Navigation Satellite Systems tropospheric products for monitoring severe weather events and climate.*

A substantial proportion of the funding, around 50% of external sources, comes from the contracts with industrial partners. The main industrial partners come from the energy sector, including major utility companies ČEZ and RWE. The collaboration has laid the foundation of a platform for both applied and theoretical research, of which some results have been mentioned above.

References

[1] Eben, Kryštof ; Resler, Jaroslav ; Juruš, Pavel ; Máj, Petr ; Pelikán, Emil. On-line System MEDARD for Weather and Air Quality Modelling And Forecasting. 2010. *www.medard-online.cz.*

[2] Konár, Ondřej ; Malý, Marek ; Brabec, Marek ; Pelikán, Emil ; Kasanický, Ivan. Spolupráce na vyhlášce o pravidlech trhu s plynem č. 370/2010 Sb. 2010.

[3] Konár, Ondřej ; Malý, Marek ; Brabec, Marek ; Pelikán, Emil ; Kasanický, Ivan. Spolupráce na vyhlášce o pravidlech trhu s plynem č. 442/2011 Sb. 2011.

[4] Konár, Ondřej ; Malý, Marek ; Brabec, Marek ; Pelikán, Emil ; Kasanický, Ivan. Spolupráce na vyhlášce o pravidlech trhu s plynem č. 436/2012 Sb. 2012.

[5] Soldo, Božidar. "Forecasting natural gas consumption." *Applied Energy* 92 (2012): 26-37.

[6] Brabec, Marek ; Paulescu, M. ; Badescu, V. Tailored vs Black-Box Models for Forecasting Hourly Average Solar Irradiance. *Solar Energy*. 2015, Roč. 111, January, s. 320-331. ISSN 0038-092X.

[7] Brabec, Marek ; Badescu, V. ; Paulescu, M. Cloud Shade by Dynamic Logistic Modeling. *Journal of Applied Statistics*. 2014, Roč. 41, č. 6, s. 1174-1188. ISSN 0266-4763.

[8] Brabec, Marek ; Paulescu, M. ; Badescu, V. Generalized Additive Models for Nowcasting Cloud Shading. *Solar Energy*. 2014, Roč. 101, March, s. 272-282. ISSN 0038-092X.

[9] Brabec, Marek ; Badescu, V. ; Paulescu, M. Nowcasting sunshine number using logistic modeling. *Meteorology and Atmospheric Physics*. 2013, Roč. 120, č. 1-2, s. 61-71. ISSN 0177-7971.

[10] Juruš, Pavel ; Eben, Kryštof ; Resler, Jaroslav ; Krč, Pavel ; Kasanický, Ivan ; Pelikán, Emil ; Brabec, Marek ; Hošek, Jiří. Estimating climatological variability of solar energy production. *Solar Energy*. 2013, 98 Part C, December, s. 255-264. ISSN 0038-092X.

[11] Paulescu, M. ; Badescu, V. ; Brabec, Marek. Tools for PV (photovoltaic) plant operators: Nowcasting of passing clouds. *Energy*. 2013, Roč. 54, č. 1, s. 104-112. ISSN 0360-5442.

[12] Resler, Jaroslav ; Eben, Kryštof ; Juruš, Pavel ; Liczki, Jitka. Inverse Modeling of Emissions and their Time Profiles. *Atmospheric Pollution Research*. 2010, Roč. 1, č. 4, s. 288-295. ISSN 1309-1042.

[13] Pappin, A. ; Hakami, A. ; Resler, Jaroslav ; Liczki, Jitka ; Vlček, O. Attribution of Ozone Pollution Control Benefits to Individual Sources. In Steyn, D.; Builtjes, P.H.; Timmermans, R.M.A. (ed.). *Air Pollution Modelling and its Application XXII*. Dordrecht : Springer, 2014, S. 41-46. ISBN 978-94-007-5576-5. ISSN 1874-6519.

[14] Kukkonen, J. ; Olsson, T. ; Schultz, D.M. ; Baklanov, A. ; Klein, T. ; Miranda, A.I. ; Monteiro, A. ; Hirtl, M. ; Tarvainen, V. ; Boy, M. ; Peuch, V.H. ; PoupKou, A. ; Kioutsioukis, I. ; Finardi, S. ; Sofiev, M. ; Sokhi, R. ; Lehtinen, K.E.J. ; Karatzas, K. ; San José, R. ; Astitha, M. ; Kallos, G. ; Schaap, M. ; Reimer, E. ; Jakobs, H. ; Eben, Kryštof. A review of operational, regional-scale, chemical weather forecasting models in Europe. *Atmospheric Chemistry and Physics*. 2012, Roč. 12, -, s. 1-87. ISSN 1680-7316.

[15] Kasanický, Ivan, Jan Mandel, and Martin Vejmelka. "Spectral diagonal ensemble Kalman filters." *arXiv preprint arXiv:1501.00219* (2014).

Research Report of the team in the period 2010–2014

Institute	Institute of Computer Science of the Czech Academy of Sciences

Scientific team	Department of Medical Informatics and Biostatistics

The team of the Department of Medical Informatics and Biostatistics is a small group of researchers combining applied research in medical informatics and biostatistics with methodological research in important tasks of computer science or mathematics. Our main aim in the period 2010–2014 can be characterized as providing a comprehensive support for interdisciplinary biomedical research with a high societal relevance.

Historically, the team was binded to the personality of Prof. RNDr. Jana Zvárová, DrSc. Thanks to her organizational talent and her ability to obtain research grants, she was able to build the medical informatics team at our institute since the beginning of 1990s. Her intention was to develop and apply tools of medical informatics and statistics to medicine. Her mission can be characterized as a desire to enrich the biomedical research and individual physicians by a variety of applied results in medical informatics and statistics. At the same time, her important activity since the very beginning was the organization of statistical courses for clinicians. Originally, these courses were organized in the English language for international participants. Currently, these courses exist in the Czech language.

In 2010–2011, most team members were active in the interdisciplinary project – Center of Biomedical Informatics (CBI), a center of applied research funded by the Ministry of Education, Youth and Sports of the Czech Republic.

Gradually, two main directions evolved, which dominate the current research of the team:

a) Biostatistical analysis of medical data,
b) Reduction of complexity of high-dimensional data.

The direction (a) was one of the major activities of the team from the very beginning in 1990s. The aim of this work is not only a statistical service for medical researchers at medical faculties or clinicians in hospitals, but a tight collaboration. Thus, the biostatistician participates in proposing the study design so that the observed data allow to formulate statistically significant results.

The orientation of the team on biostatistics became prevalent at the beginning of 2012 after the end of CBI, when only the core researchers remained at the institute. Then, the name of the team (at that time Department of Medical Informatics, DMI) was extended to Department of Medical Informatics and Biostatistics (DMIB).

The direction (b) was motivated by our practical experience in analysing molecular genetic data. We realized that standard methods of multivariate statistics are not suitable if the number of observed variables p exceeds the number of observations n. Nevertheless, it is a typical situation in molecular genetics that there are thousands or tens of thousands of variables (gene expressions) measured on a sample of tens or hundreds of patients. Typically, the aim of the analysis is to learn a classification rule allowing to assign a new individual to one of several different classes, e.g., according to the diagnosis. Standard methods of both statistics and data mining suffer from the so-called curse of dimensionality for such high-dimensional data, which is revealed through numerical instability or computational infeasibility. Although it is possible to reduce the complexity of the data by a prior variable selection, preferable approaches seem to employ a suitable regularization to obtain modified (regularized) versions of standard classification methods, which have been investigated and applied by our team.

A. Cardiovascular Genetic Study

A major result of the research of the team in the period 2010–2014 was a large cardiovascular genetic study, unique within the Czech Republic. The aim of this interdisciplinary research was to find a small set of genes responsible for the diagnosis and prognosis of cardiovascular diseases. We played a crucial role in preparing the design of this matched case-control study on 181 individuals. Peripheral blood samples of patients were matched to those of control persons based on risk factors. The patients were investigated again six months after the myocardial infarction and the survival status of the patients was used to identify two distinct subgroups.

Our team members performed extensive statistical evaluations of the results of the whole cardiovascular genetic study. The classification methods used on the high-dimensional genetic data are based on the shrinkage statistical estimation, which has obtained recent attention in the analysis of data in molecular genetics. These include a shrinkage version of linear discriminant analysis and a linear model for microarray data (limma). A predictive analysis of the data allowed us to find sets of differentially expressed genes with predictive properties in independent samples. We evaluated the predictive properties using bootstrap sampling.

Within the study, we identified genes associated with excess genetic risk of acute myocardial infarction, including those associated with the six months fatality of the cases. Further, we described a method for evaluating expression intensities of 10 selected genes in a biological sample taken from the body of patients. The method allows to identify individuals with a higher genetic risk of death in consequence of cardiovascular complications within 6 months from the occurence of an acute myocardial infarction. These applied results of the genetic study within CBI allowed us to obtain four national patents (e.g. [1]) and a utility model and are described in publications (e.g. [2]).

B. E-health

One important task of medical informatics is to propose and implement tools of electronic health care (e-health), reflecting the needs of hospitals or individual clinicians.

First, we proposed and implemented a prototype of a system for clinical decision support [3]. Generally speaking, clinical decision support systems offer an aid in the decision making process in various areas. In clinical medicine, they represent a modern e-health tool with the ability to assist in finding a diagnosis, therapy and prognosis of patients. Our internet classification service abbreviated as SIR (System for Selecting Relevant Information for Decision Support) is a tool for the statistical analysis within a clinical study even in a situation with a very large number of medical symptomes being observed. It allows to select such symptomes (variables), which are the most relevant for determining the diagnosis. Thus, knowledge from research can spread easily and quickly to clinicians, who may use the support during their decision making. We tested the prototype of the system on the cardiovascular genetic study mentioned above. The result [3] was awarded as the best scientific paper of the year 2013 by the Czech Society for Biomedical Engineering and Medical Informatics.

Further, we proposed and implemented a system of structured voice-supported data entry in the electronic health record in the field of dentistry. The prototype of the structured electronic health record extended our previous prototypes for Czech healthcare called MUDR (Multimedia-Distributed Electronic Health Record) and MUDRLite. The architecture of the prototype revealed advantages of structured data entry for an electronic health record application in temporo-mandibular joint disorders.

We used international standards and nomenclatures for building a pilot interoperability platform that should serve to exchange information among electronic health record systems in Czech healthcare. We also discussed semantic interoperability requirements for a nationwide implementation of HL7 version 3 into the Czech electronic healthcare.

Finally, we focused on investigating narrative medical reports. Their terminology is far from being standardized and thus they cannot provide sufficient information for medical decision making needed in electronic healthcare. We proposed a method for measuring diversity in medical reports written in any language to compare diversities in narrative and structured medical reports and to map attributes and terms to selected classification systems. We applied the new method based on the information theory to Czech narrative or structured medical reports. The results contribute to the theoretical framework for developing future text mining procedures tailor-made for narrative medical reports.

C. Statistical Analysis of Data in Medicine

An important part of the applied research of the team can be described as the analysis of biomedical data by means of biostatistical methods. Modern biostatistical methods are intensively applied to various areas of clinical medicine, including Dentistry, Gastroenterology, Physiology, Otorhinolaryngology, Clinical neurology, Neuro-sciences, or Molecular Genetics.

The contribution of our team members to these areas was the statistical part of the research, including the design of the study, the choice of a suitable statistical methodology, and the analysis of the data. In other words, the aim of our work in this area was to extract information from biomedical data and their correct interpretation within the biomedical problem.

In the period 2010-2014, we continued maintaining a software application for collecting cardiological data into a register of acute coronary syndromes ALERT-CZ. Its name is an abbreviation of Acute Coronary Syndromes – Longitudinal Evaluation of Real-life Treatment in Non-PCI Hospitals in the Czech Republic. Until 2011, we devoted ourselves to the biostatistical analysis of the data stored in the register. The whole project was organized by the Third Faculty of Medicine of Charles University in Prague under the auspices of the Czech Cardiological Society.

D. Mathematical Statistics

Hypothesis testing represents a basic statistical tool for the analysis of data, particularly important for the analysis of multivariate data in biomedicine. We were involved in methodological research in the area of nonparametric statistics. Because various existing tests are not necessarily finite-sample unbiased, we investigated nonparametric statistical tests for comparing the equality of distribution between two random samples of multivariate data. It has been known for a long time that various existing tests may have a very low power. Under the alternative hypothesis, the power is even below 5 %. This is true also for one-dimensional as well as for multivariate data. So far, the problem had not attracted any attention for the more complicated case of multivariate data. We proposed several new multivariate tests [5], which are based on distances of observations from a certain given or randomly selected point. The new methods include a multivariate Wilcoxon test. In other words, we generalized the most commonly used nonparametric statistical method to the multivariate setting. We showed suitable properties (including the optimality) of newly proposed tests under general assumptions and investigated their computational aspects.

E. Image Analysis

Our research in the area of image analysis aimed at proposing and implementing robust image analysis procedures, which are insensitive to the presence of noise and outlying values in the images [6]. These methods include a new robust correlation coefficient. It has a high breakdown point, i.e., it is resistant to a larger percentage of severe outliers in the data. We derived theoretical properties (e.g. robustness and asymptotic behavior) of the new correlation coefficient, which turns out to be computationally stable. At the same time, it allows a clear interpretation in accordance with intuition. The tasks of face localization and face recognition in a database of real images allowed us to reveal the superiority of robust methods compared to their standard counterparts [6], particularly in images contaminated by severe noise.

Moreover, we carried out face localization by detecting symmetric areas in the images. In this applied study, robust measures of similarity between two images turn out to be the best methods for measuring symmetry in faces. The method implemented in this applied research is resistant with respect to noise in the image, occlusion in the face, or to asymmetric hair style. It is able to detect the rather delicate asymmetric illumination in the background, while standard methods are masked by outliers and intrigued by the asymmetry in the background. The hair, shoulders, or collar are generally asymmetric and violate the assumption of symmetry of the image, although the face itself is relatively symmetric. The implicitly weighted robust correlation coefficient assigns small weights to these asymmetric parts of the face and turns out to yield reliable results in the face localization task. This is an argument in favor of using the robust statistical methodology in image analysis tasks.

F. Other Research Topics

Other topics investigated by members of the team included

- Forensic genetics,
- Biometric identification in biomedicine,
- Electronic information sources in biomedicine.

Research Grants

The list of research grants for the period 2010-2014 with the main researcher from our team includes two grants from public sources:

Project title	Main researcher	Identification number from Appendix 3.1	Years
Center of Biomedical Informatics	Zvárová	33	2006-2011
Role of folates in pathogenesis of metabolic syndrom	Zvárová	34	2009-2011

In addition, one prestigious research grant comes from private sources:

Project title	Main researcher	Years	Funding	Panel
Robust analysis of high-dimensional data	Kalina	2014-2016	Neuron Fund for Support of Science	Mathematics

International Collaboration

Currently, P. Martinková from our team is at the University of Washington in Seattle, at the Department of Statistics. She is there for two years (2013–2015), while she was a Fulbright researcher in the first year and is a visiting research scholar in the second year.

Numerous memberships of team members in international scientific societies and commissions are described in detail in Appendix 3.10.

Textbooks

Besides numerous scientific results, our team members were participating in writing several monographs for graduate students of medicine. Monographs in the Czech language were written during 2010-2014 on the following topics:

- Molecular bioinformatics [7],
- Processing data and knowledge in biomedicine [8],
- Construction of educational tests [9].

J. Zvárová was the main author of the books [7] and [8]. P. Martinková was one of several authors of the book [9].

Selected References

[1] **Zvárová** J. – Mazura J. – **Valenta** Z. – Feglarová P. – Grünfeldová H. (2012): *Method for identifying persons with increased genetic risk of decrease after myocardial infarction.* Patent of the Czech Republic No. 303458, date of patent publication 19.9.2012.

[2] **Valenta** Z. – Mazura I. – Kolář M. – Grünfeldová H. – Feglarová P. – Peleška J. – Tomečková M. – **Kalina** J. – **Slovák** D. – **Zvárová** J. (2012): Determinants of excess genetic risk of acute myocardial infarction - a matched case-control study. *European Journal for Biomedical Informatics* 8 (1), 34-43.

[3] **Kalina** J. – Seidl L. – **Zvára** K. – Grünfeldová H. – **Slovák** D. – **Zvárová** J. (2013): System for selecting relevant information for decision support. *Studies in Health Technology and Informatics* 186, 83-87.

[4] Kříž P. – Seydlová M. – Dostálová T. – **Valenta** Z. – Chleborád K. – **Zvárová** J. – Feberová J. – Hippmann R. (2012): Dental implants and improvement of

oral health-related quality of life. *Community Dentistry and Oral Epidemiology* 40, Suppl. 1, 65-70.

[5] Jurečková J. – **Kalina** J. (2012): Nonparametric multivariate rank tests and their unbiasedness. *Bernoulli* 18 (1), 229-251.

[6] **Kalina** J. (2012): Implicitly weighted methods in robust image analysis. *Journal of Mathematical Imaging and Vision* 44 (3), 449-462.

[7] **Zvárová** J. – Mazura I. – Bendlová B. – **Kalina** J. – Kolář M. – Krylov V. – Lukeszová L. – Mácha J. – Rídl J. – Schneider B. – Strnad H. – Ulbrich P. – Vajdová E. – **Valenta** Z. – Včelák J. (2012): *Methods of molecular biology and bioinformatics*. Karolinum, Praha. (In Czech.)

[8] **Zvárová** J. – Lhotská L. – Přibík V. – Adášková J. – Brechlerová D. – Hanzlíček P. – Huptych M. – Kopecký M. – **Papíková** V. – Potůček J. – **Přečková** P. – Říha A. – Svátek V. – Šárek M. – Zitová B. – **Zvára** K. (2010): *Data and Knowledge in Biomedicine and Healthcare*. Karolinum, Praha. (In Czech.)

[9] Štuka Č. – **Martinková** P. – Vejražka M. – Trnka J. – Komenda M. (2013): *Student Assessment in Medical Education. Construction and Analysis of Tests at Medical Faculties.* Karolinum, Praha. (In Czech.)

Research Report of the team in the period 2010–2014

Institute	Institute of Computer Science of the Czech Academy of Sciences

Scientific team	Department of Nonlinear Dynamics and Complex Systems

The search for order in chaos, reflecting complex phenomena in nature and society, is a challenge attracting researchers from various areas of science and technology. The new field of nonlinear dynamics and theory of complex systems emerges in interactions of mathematics, physics and computer science. The team of the Department of Nonlinear Dynamics and Complex Systems, recently established within the Institute of Computer Science (ICS), is gradually gaining international recognition in the effort to use and creatively develop ideas from the theory of nonlinear dynamical systems, deterministic chaos and information theory in order to design mathematical methods and computer algorithms suitable for the analysis of multivariate time series reflecting complex dynamics of various origins, ranging from the atmospheric phenomena to the activity of the human brain.

To give an example, the abstract meaning of the "search for order in chaos" can be translated into the language of everyday life considering question such as "Why the last winter (in Central Europe) was so warm and will the next one be similar or colder? Should I buy ski equipment, or how expensive will be my next energy bill?" The Earth atmosphere with variable weather and changing climate is a typical complex system. In general, complex systems evolve on multiple time scales. Do the dynamics on different time scales evolve independently, or do they mutually interact, influence each other? For answering such questions, in [1] we have developed an information-theoretic approach to detection of information transfer between dynamical phenomena evolving on different time scales of a complex multiscale process - such as the dynamics of the Earth atmosphere. Analysing long-term records of air temperature from various European locations, we have uncovered an information transfer in a form of a causal relation between the phase of slow irregular oscillations, mainly with the period of about 7-8 years, and the amplitude of faster temperature fluctuations occurring on time scales of a few weeks to 2-3 years.

Such cross-scale interactions are known in brain dynamics; however, for the atmospheric physics it is a newly discovered phenomenon. In order to understand its significance, we remind that irregular cycles with various periods have been observed in the changing Earth climate. While the El Niño phenomenon occurring with the period of about 3-6 years is well known, the cycle with the period of about 7-8 years detected in the climate-related data is still a subject of interest for a narrow circle of researchers. The amplitude of the 7-8-year cycle is relatively low and the cycle is hidden in complex, noise-like climate variability. Consequently this cycle was not yet considered in climate change studies, nor in comprehensive climate models. However, as a consequence of the observed cross-scale information transfer, the overall effect of these slow oscillations on the inter-annual temperature variability can reach the range of 1-2 degrees Celsius in large areas of Europe. Such changes in annual mean temperature can have considerable effects on our everyday lives.

Main research directions

The search for order in chaos entails an effort to understand complex and complicated behaviour of real-world phenomena, recorded in time-dependent experimental data, time series. In this endeavour we can specify the following main research directions:

(1) Detection of nonlinear phenomena

Is it just an unpredictable noise, or is there a more regular variability or a repeating pattern hidden in a noise background? It is a typical question of researchers facing recordings of complex processes such as the brain activity or a long-term recording of the air temperature. Within this research direction, we develop and apply **original tests for nonlinearity in time series**, and algorithms for detecting nonlinear oscillations hidden in a background of nontrivial noise. Besides the detection, researchers are interested also in the characterization of nonlinear phenomena, in particular in the **quantitative characterization of complexity** of studied process. Concepts based on the notion of entropy and entropy rates have been developed and applied.

(2) Interactions in complex systems:

"More is different," this simple sentence of the Nobel laureate physicist P. W. Anderson reflects the complex reality in which the behaviour of complex systems, consisting of many interacting elements, cannot be explained by a simple extrapolation of the laws describing the behaviour of a few elements. In order to understand complex systems we need to identify and describe interactions of their elements. Interacting complex systems can be coupled, can communicate and exchange information and, eventually, they can reach a high level of cooperative behaviour – synchronization. The team works on the development of reliable methods and algorithms for the identification of various cooperative phenomena from time series recording evolution of complex systems. The team had the unique opportunity to further develop original results obtained before the evaluated period: M. Paluš has proposed the first quantitative method for the detection of phase synchronization [2] and a concept of synchronization as adjustment of information rates [3]. The latter work uses tools from information theory in order to **detect synchronization and causality** (in the Granger sense) from time series of interacting dynamical systems. Information-theoretic approaches for detection of causality from time series, developed by M. Paluš and collaborators, have gained international recognition, documented by high citation counts of the papers [4,5,6].

Dynamics of complex systems is frequently reflected in measurements of many variables or a few variables in many spatial locations. Therefore **multidimensional data reduction and clustering** is also one of the research topics of this team.

Interactions of many elements are recently modelled and studied as **complex networks**.

(3) Modelling emergent phenomena in complex dynamics

Interactions of many subsystems within a complex system commonly lead to a qualitatively different behaviour from that manifested by isolated subsystems. Understanding the mechanisms of emergence of this qualitatively different behaviour goes beyond the detection of the interactions, as the interactions may lead to the emergence of new phenomena only under specific circumstances. One of the most fascinating area of study of emergent phenomena is neuroscience. Some of the questions that we study are: What is the mechanism of emergence (and disappearance) of epileptic seizure from normal electrophysiological activity? What is the role of altered inhibition, excitation, or structure of brain network connections? To what extent are the brain activity dynamics constrained by the relatively fixed structural connections between the brain areas?

(4) Data mining and evolutionary optimization is a research direction complementing the above described research areas, both in theoretical development and in applications. The general aim is the extraction of knowledge from data; or discovering patterns. In the recent period, our research focused mainly on three areas: the extraction of rules of an observational calculus, the detection and explanation of anomalies and evolutionary optimization.

Main results for the evaluated period 2010-2014

The results can be attributed to particular projects and also to the above defined main research directions. The latter attribution, however, is not always unambiguous, since some research topics may overlap, or one research topic naturally emerges from another.

(1) Detection of nonlinear phenomena

In the field of **Detection of nonlinear phenomena**, the team amended the question of existence of nonlinearity by a quantification of its effects. The role of nonlinearity has been assessed in multivariate neural data [7,8] and in studies of interactions in the atmospheric dynamics [9]. The obtained results develop the field of **Interactions in complex systems**, including the problem of construction of **complex networks**, in particular brain networks and climate networks.

Another direction within the field of **Detection of nonlinear phenomena** is the **detection of oscillatory phenomena in a nontrivial noise** (so called red or pink noise) background. In the reported period, Vejmelka et al. [10] have developed a method grounded in nonlinear dynamics to detect whether nonlinear oscillatory activity of a certain frequency range can be reliably detected in a broadband time series (such as the human EEG). The method is a fresh approach to distinguishing linear stochastic processes from nonlinear oscillatory processes that is based on a careful statistical analysis.

The area of **characterization of complex dynamics** has found applications in the reported period within the cooperation with neuroscientists. Epilepsy is the second most common neurological disease (after stroke) and affects approximately 1% of the population in developed countries. The current treatment of epilepsy is long-term, lasting years or even for the patient's whole lifetime. In around 25% of patients medical therapy is ineffective and presents a substantial disease burden. The main disabling factor of epilepsy is seemingly sudden and random occurrence of seizures.

Therefore, how seizures start is a major question in epilepsy research. The study [11] (which has already obtained 56 WoS citations) demonstrates the existence of a preictal state characterized by an increase in neuronal activity associated with a widespread buildup of a low-amplitude high-frequency activity (HFA) and a reduction in system complexity. The rapid expansion and fusion of the neuronal populations responsible for HFA, and a progressive slowing of HFA, leads to a single hypersynchronous cluster generating the high-amplitude low-frequency activity of the seizure. M. Paluš contributed to this study by the quantification of the system complexity in terms of entropy rates, using the mathematical methods and algorithms developed in his previous research [12,13].

(2) Interactions in complex systems

When investigating **Interactions in complex systems,** the need for solutions for **multidimensional data reduction and clustering** naturally emerges. Vejmelka and Paluš [14] report on a method for exploratory data analysis that automatically picks out elements from a group that exhibit an increased connectivity to each other as estimated from time series recordings. It defines and builds on the concept of cluster strength and it employs eigenvalue/eigenvector analysis of the connectivity matrix to determine which elements should be assigned to clusters and which form a "remainder" or a residual.

The definition of key modes of the variability explaining the global atmospheric dynamics is a central climatological question. To this purpose, we have developed a principled approach based on a combination of rotated PCA decomposition and the comparison of the eigenspectrum to its empirical null distribution. In particular, for the null distribution we proposed to use a surrogate model used in the nonlinear dynamics community for different purposes, namely of independent stochastic processes replicating the auto-correlation structure of each time series [15].

Interactions in complex systems consisting of many components are recently modelled using **complex networks**. Of particular importance are the complex networks constructed from multivariate time series. The team effort contributed to the solution of critical questions of the network construction, namely to the choice between linear and nonlinear dependence measures [7,8,9] and to the understanding how the properties of dependence measures influence the complex network topology [16,17]. Here we can see how the same mathematical concept can be useful in different areas of science. The papers [7,8] are results of the project [P1] and solve the problems of the construction of brain networks. The study [7] introduces a method for the quantification of deviations of functional connectivity from linearity. The application to resting state functional magnetic resonance imaging data shows that the functional connectivity is almost perfectly linear. This provides a game-changing quantitative argument for the use of efficient linear correlation estimators for functional connectivity; an intuitive practice being earlier challenged by the proponents of sophisticated, but often less efficient, nonlinear methods. On the other hand, the paper [8] introduced a framework for detection of influence of nonlinear connectivity between subsystems on the global complex network analysis; apart from the current application to the brain it is of relevance for researchers in other complex network application fields.

The studies [7,8] are results of an international collaboration within the FP7 project BrainSync [P1]. The ICS team (Hartman, Hlinka, Paluš, Vejmelka) designed the methods and algorithms, programmed the computer codes and performed the analyses. The international co-authors provided the data and discussed the relevance of results using their neuroscience know-how.

The papers [9,16,17] are results of the project [P2] and are related to fundamental problems of construction and the interpretation of climate networks, which are used as a mathematical abstraction of interactions of many intertwined physical processes influencing atmospheric dynamics and climate evolution. Representing a continuous spatio-temporal phenomenon as a subject of discrete mathematics leads to a reduction of information. A climate network (a directed or undirected graph) should be constructed from measured data in such a way that it reflects underlying physical processes and their interactions. In [17] we demonstrate a common bias in used connectivity measures and further show that properly inferred network links build climate networks reflecting known phenomena of climate variability such as El Nino, North Atlantic Oscillation, or external influences such as the variability of the solar activity.

The paper [9] introduces a method for the systematic study of nonlinear dependence structures in climate data, including their geographical and temporal distribution. An example analysis in monthly temperature data shows only weak nonlinearity; most of which we could attribute to specific artificial sources. This gives the first objective support for the use of the most precise linear dependence estimators. Community response suggests this is a key finding affecting methodology in the climate network research.

The study [16] points out and explores an important graph-theoretical property of correlation matrices – the increased occurrence of so-called small-world structure in binarized correlation graphs, compared to random graphs of the same size and edge density. This observation sheds new light on observations of small-world properties of correlation graphs of many complex systems including brain and climate, suggesting these may not be a specific property of the systems, but an artifact of the method. Importantly, many complex dynamical systems are also nonstationary, with the pattern of depedencies between the subsystems changing over time. In [18] we have studied in detail the evolution of the global temperature network structure over second half of the twentieth century.

When assessing **interactions** it is not only important to find which system parts are mutually dependent or synchronized, but also to identify which element (subsystem) is influencing which. The concept of Granger causality, previously extended to nonlinear systems using information-theoretic functionals, was applied in order to study **causal interactions** in the climate system and in the construction of directed climate networks. In the study [19] the linear Granger causality analysis as a tool for discovering the climate networks was compared with two most common nonlinear methods, each of which was tested using a representative range of implicit parameter settings. The analysis showed quantitatively that linear Granger causality analysis outperforms in reliability the nonlinear counterparts on real data, as well as the role of parameter choices. The result is now routinely considered in the climate networks community in method selection.

The papers [18,19] resulted also from international cooperation within the project [P2]. The ICS team (Hartman, Hlinka, Paluš, Vejmelka) designed the methods and algorithms, programmed the computer codes and performed the analyses. The German co-authors helped to interpret the results within the field of climate networks.

The method which detects causal relations and information flows in multiscale systems [1] has already been described in the introduction of this report. It led to discovering a new phenomenon in atmospheric dynamics, which is under intensive research of our team and international collaborators in Germany and the USA.

(3) Modelling emergent phenomena in complex dynamics

Interactions of parts of complex systems often give rise to novel coherent structures, patterns and properties observable at the system level. In many cases it is the existence and stability of these emergent phenomena that is of key interest for the specific field. Therefore, understanding the conditions under which such emergence occurs and a possible mechanism thereof form an important contribution of computational sciences to other fields of knowledge. To gain such understanding, a combination of theoretical analysis and numerical simulations of models of the complex systems of interest needs to be carried out.

For example, in human brain, the activity of specific pairs of distant neural populations is synchronized, forming a matrix of so-called functional connectivity of brain areas. The emergence and maintenance of effective synchronization pattern is key for healthy brain function. Such synchronization is enabled by the underlying physical connections between brain areas via neural axon fiber bundles. However, such structural connectivity itself is insufficient to explain the emerging functional connectivity. In a semi-analytic study [20] we have documented the importance of the parameters of intrinsic local and coupling dynamics of the neural populations, pointing towards a critical role of a particular metaparameter, related to pairwise synchronizability. While building on an ongoing collaboration with the University of Nottingham UK, the research is being further developed in project [P6] and within the collaboration with the National Institute of Mental Health in Klecany, Czech Republic, providing rich data for model validation.

We also work on the formulation of models for key phenomena in other neuroscience fields: the initiation, dynamics, and termination of epileptic seizures (project [P3]), or the neuronal models of the emergence of musical tonality, i.e. the perceived hierarchy among tones in music. In contrast, we have applied a phenomenological modelling strategy to show that some prominent patterns in data emerge as a result of commonly unsuitable adopted data analysis or interpretation strategies – this was shown for instance for the case of small-world structure of functional connectivity networks [16], or in a very recently published study on dangers of brain nonstationarity detection [21].

In 2014, we have started a work in the direction of modelling emergence of important phenomena in climate dynamics, such as the existence and dynamics of teleconnections – non-local synchronization of pressure and temperature fields.

(4) Data mining and evolutionary optimization develops in basic and oriented applied research directions.

In the area of research in **data mining**, two directions were pursued.

The first is the extraction from data of **rules of an observational calculus** with generalized quantifiers based on hierarchical Archimedean copulas. Copulas allow separating marginals from the structure connecting them. At the same time, using copulas allows extracting rules from data governed by continuous distributions, without a preceding discretization that typically decreases the accuracy of the resulting rules. Finally, hierarchical Archimedean copulas share many features with classification trees. Apart from several conference papers, our main results in this direction of research are a journal paper and a book chapter published in the Springer series Lecture Notes in Artificial Intelligence [22,23].

The second direction pursued is the detection and **explanation of anomalies** by means of random forests. The detection of anomalies is a classification task belonging to those tasks in which the comprehensibility of the result of classification is very important. We combine existing methods of anomaly detection with specific random forests consisting of a small number of classification trees. Using rules extracted from those trees, a comprehensible explanation of the anomaly can be obtained. This direction of research started only in mid 2013, that is why it brought only workshop papers so far, e.g. [24], but the results are quite promising.

In the area of research in **evolutionary optimization**, we focused on the use of **surrogate models** in evolutionary optimization. A surrogate model is a regression model employed in optimization as a replacement of the evaluation of the true objective function if that evaluation is expensive or incurs high computational costs. We pay a specific interest to Gaussian process-based surrogate models, for two reasons: first, they have been already successfully used outside evolutionary optimization; second, they differ from most other regression models through the attractive ability to provide not only a point estimate of the true objective function, but also the estimate of the distribution of its function values. So far, our research in this direction brought a number of conference papers, including papers in high quality conferences such as GECCO or IDEAL [25,26].

In the assessed period, most applications of these data mining techniques were in the area of **a search for new catalytic materials.** For oxidative coupling of methane, data mining of experimental data from testing the performance of many hundreds of different catalysts was performed. Its results provide new insights into the catalysis of the respective reaction, but also contribute to the methodology of research in this area [27]. In addition, data from the analysis of hundreds of catalysts for high-temperature synthesis of hydrocyanic acid performed during 2004-2007 [28] were reanalysed with additional methods not used during the original analysis [29]. Also, a system for evolutionary optimization of catalytic materials, under development since 2005, was finished in 2011. In that system, some results of the research into surrogate modelling were incorporated [30].

Concluding remarks

The above reported results were sorted into four research directions characteristic for the team of the Department of Nonlinear Dynamics and Complex Systems. These results were published in different journals – the number of journal categories (WoS classification) is about ten, ranging from computer science, applied mathematics and multidisciplinary physics through physical chemistry, geochemistry and geophysics, meteorology and atmospheric sciences to neuroimaging and neurosciences. The reason for this heterogeneity is the interdisciplinary character of the research in the area of complex systems. Complexity in different scientific disciplines has, in many cases, common general principles. Therefore, the same mathematical principles and computer algorithms help to understand complex behaviour in different areas. This team is active in both principal directions of complexity research – in the development of mathematical methods and computer algorithms and in their applications in basic research of diverse fields from atmospheric physics to neuroscience. One research area in the methods development is the identification of causal interactions from complex time series. In this area the team has joined the world-leading scientific teams, setting research directions and standards, already in the previous evaluation period - the three papers [4, 5, 6] published in 2007 and 2008 have been recognized internationally and together have obtained over 320 WoS citations. In the evaluated period 2010-2014 this research direction developed into two branches: the first branch is the construction of complex networks from multivariate time series – the principal problems of interaction networks inference were solved in papers [7, 8] devoted to the brain networks, in papers [9, 17, 18, 19] focused to the climate networks and the paper [16] deals with the small-world topology of complex networks in general. Together these publications have attracted about 100 (97 in April 2015) WoS citations and the approaches proposed become parts of method sections in recent publications of independent complexity researchers worldwide. The second branch of the causality research is the cross-scale information transfer introduced in the letter [1]. This is generally a new research direction; we expect its intensive development in the coming years.

Projects

[P1] 2008–2011 FP7 project BrainSync – Large scale interactions in brain networks and their breakdown in brain diseases (FP7-HEALTH 200728)

[P2] 2011–2013 Czech Science Foundation project No. P103/11/J068: Interactions, information transfer and complex structures in the dynamics of changing climate. Bilateral project with the Potsdam Institute for Climate Impact Research

[P3] 2014–2016 Czech Science Foundation project No. 14-02634S: Large-scale dynamics and critical transitions in neuronal networks and their role in limbic seizure genesis

[P4] 2014–2016 MEYS CR program KONTAKT II project LH14001: Climate networks: Multiple scales of dynamics and interactions in the Earth atmosphere, with University of Wisconsin-Milwaukee

[P5] 2013-2015 Czech Science Foundation project No. 13-17187S, Constructing advanced comprehensible classifiers.

[P6] 2013-2015 Czech Science Foundation project No. 13-23940S, Personality and spontaneous brain activity during rest and movie watching: relation and structural determinants

References

[1] M. Palus, Multiscale atmospheric dynamics: Cross-frequency phase-amplitude coupling in the air temperature, PHYSICAL REVIEW LETTERS, vol. 112, no. 7, 2014.

[2] M. Palus, Detecting phase synchronization in noisy systems, PHYSICS LETTERS A, vol. 235, no. 4, pp. 341-351, 1997.

[3] M. Palus, V. Komarek, Z. Hrncir, and K. Sterbova, Synchronization as adjustment of information rates: Detection from bivariate time series, PHYSICAL REVIEW E, vol. 63, no. 4, 2, pp. art. no.046211, 2001.

[4] K. Hlavackova-Schindler, M. Palus, M. Vejmelka, and J. Bhattacharya, Causality detection based on information-theoretic approaches in time series analysis, PHYSICS REPORTS-REVIEW SECTION OF PHYSICS LETTERS, vol. 441, no. 1, pp. 1-46, 2007.

[5] M. Palus and M. Vejmelka, Directionality of coupling from bivariate time series: How to avoid false causalities and missed connections, PHYSICAL REVIEW E, vol. 75, no. 5, 2, 2007.

[6] M. Vejmelka and M. Palus, Inferring the directionality of coupling with conditional mutual information, PHYSICAL REVIEW E, vol. 77, no. 2, 2, 2008.

[7] J. Hlinka, M. Palus, M. Vejmelka, D. Mantini, and M. Corbetta, Functional connectivity in resting-state fMRI: Is linear correlation sufficient? NEUROIMAGE, vol. 54, no. 3, pp. 2218-2225, 2011.

[8] D. Hartman, J. Hlinka, M. Palus, D. Mantini, and M. Corbetta, The role of nonlinearity in computing graph-theoretical properties of resting-state functional magnetic resonance imaging brain networks, CHAOS, vol. 21, no. 1, 2011.

[9] J. Hlinka, D. Hartman, M. Vejmelka, D. Novotna, and M. Palus, Non-linear dependence and teleconnections in climate data: sources, relevance, nonstationarity, CLIMATE DYNAMICS, vol. 42, no. 7-8, pp. 1873-1886, 2014.

[10] M. Vejmelka, M. Palus, and K. Susmakova, Identification of nonlinear oscillatory activity embedded in broadband neural signals, INTERNATIONAL JOURNAL OF NEURAL SYSTEMS, vol. 20, no. 2, pp. 117-128, 2010.

[11] P. Jiruska, J. Csicsvari, A. D. Powell, J. E. Fox, W.-C. Chang, M. Vreugdenhil, X. Li, M. Palus, A. F. Bujan, R. W. Dearden, and J. G. R. Jeferys, High-frequency network activity, global increase in neuronal activity, and synchrony expansion precede epileptic seizures in vitro, JOURNAL OF NEUROSCIENCE, vol. 30, no. 16, pp. 5690-5701, 2010.

[12] M. Palus, Coarse-grained entropy rates for characterization of complex time series, PHYSICA D-NONLINEAR PHENOMENA, vol. 93, no. 1-2, pp. 64-77, 1996.

[13] M. Palus, On entropy rates of dynamical systems and Gaussian processes, PHYSICS LETTERS A, vol. 227, no. 5-6, pp. 301-308, 1997.

[14] M. Vejmelka and M. Palus, Partitioning networks into clusters and residuals with average association, CHAOS, vol. 20, no. 3, 2010.

[15] M. Vejmelka, L. Pokorna, J. Hlinka, D. Hartman, N. Jajcay, and M. Palus, Non-random correlation structures and dimensionality reduction in multivariate climate data, CLIMATE DYNAMICS, vol. 44, no. 9-10, pp. 2663-2682, 2015.

[16] J. Hlinka, D. Hartman, and M. Palus, Small-world topology of functional connectivity in randomly connected dynamical systems, CHAOS, vol. 22, no. 3, 2012.

[17] M. Palus, D. Hartman, J. Hlinka, and M. Vejmelka, Discerning connectivity from dynamics in climate networks, NONLINEAR PROCESSES IN GEOPHYSICS, vol. 18, no. 5, pp. 751-763, 2011.

[18] J. Hlinka, D. Hartman, N. Jajcay, M. Vejmelka, R. Donner, N. Marwan, J. Kurths, and M. Palus, Regional and inter-regional effects in evolving climate networks, NONLINEAR PROCESSES IN GEOPHYSICS, vol. 21, no. 2, pp. 451-462, 2014.

[19] J. Hlinka, D. Hartman, M. Vejmelka, J. Runge, N. Marwan, J. Kurths, and M. Palus, Reliability of inference of directed climate networks using conditional mutual information, ENTROPY, vol. 15, no. 6, pp. 2023-2045, 2013.

[20] J. Hlinka and S. Coombes, Using computational models to relate structural and functional brain connectivity, EUROPEAN JOURNAL OF NEUROSCIENCE, vol. 36, no. 2, pp. 2137-2145, 2012.

[21] J. Hlinka and M. Hadrava, On the danger of detecting network states in white noise, FRONTIERS IN COMPUTATIONAL NEUROSCIENCE, vol. 9, 2015.

[22] J. Gorecki and M. Holena, Structure determination and estimation of hierarchical archimedean copulas based on kendall correlation matrix, in NFMCP 2013 (A. Appice, M.

Ceci, C. Loglisci, G. Manco, E. Masciari, and Z. Ras, eds.), vol. 8399 of Lecture Notes in Articial Intelligence, pp. 132-147, SPRINGER-VERLAG BERLIN, 2014. 2nd International Workshop on New Frontiers in Mining Complex Patterns (NFMCP), Prague, CZECH REPUBLIC, SEP 27, 2013.

[23] J. Gorecki, M. Hofert, and M. Holena, An approach to structure determination and estimation of hierarchical archimedean copulas and its application to bayesian classication, Journal of Intelligent Information Systems, pp. 1-39, 2015.

[24] M. Kopp, T. Pevny, and M. Holena, Interpreting and clustering outliers with sapling random forests, in ITAT 2014. Information Technologies - Applications and Theory. Part II. (V. Kurkova, L. Bajer, L. Peska, R. Vojtas, M. Holena, and M. Nehez, eds.), pp. 61-67, Institute of Computer Science AS CR, 2014.

[25] L. Bajer and M. Holena, Surrogate model for continuous and discrete genetic optimization based on rbf networks, in IDEAL 2010 (C. Fyfe, P. Tino, D. Charles, C. GarciaOsorio, and H. Yin, eds.), vol. 6283 of Lecture Notes in Computer Science, pp. 251-258, SPRINGER-VERLAG BERLIN, 2010. 11th International Conference on Intelligent Data Engineering and Automated Learning, Univ W Scotland, Paisley, SCOTLAND, SEP 01-03, 2010.

[26] M. Holena, D. Linke, and L. Bajer, Surrogate modeling in the evolutionary optimization of catalytic materials, in PROCEEDINGS OF THE FOURTEENTH GECCO (T. Soule, ed.), pp. 1095-1102, SIGEVO ACM Special Interest Grp Genet & Evolutionary Computat, ASSOC COMPUTING MACHINERY, 2012. 14th International Conference on Genetic and Evolutionary Computation Conference (GECCO), Philadelphia, PA, JUL 07-11, 2012.

[27] U. Zavyalova, M. Holena, R. Schloegl, and M. Baerns, Statistical analysis of past catalytic data on oxidative methane coupling for new insights into the composition of high-performance catalysts, CHEMCATCHEM, vol. 3, no. 12, pp. 1935-1947, 2011.

[28] S. Moehmel, N. Steinfeldt, S. Engelschalt, M. Holena, S. Kolf, A. Baerns, U. Dingerdissen, D. Wolf, R. Weber, and M. Bewersdorf, New catalytic materials for the high-temperature synthesis of hydrocyanic acid from methane and ammonia by high-throughput approach, APPLIED CATALYSIS A-GENERAL, vol. 334, no. 1-2, pp. 73-83, 2008.

[29] M. Holena, N. Steinfeldt, M. Baerns, and D. Stefka, Computing the correlation between catalyst composition and its performance in the catalysed process, COMPUTERS & CHEMICAL ENGINEERING, vol. 43, pp. 55-67, 2012.

[30] M. Holena, D. Linke, and U. Rodemerck, Generator approach to evolutionary optimization of catalysts and its integration with surrogate modeling, CATALYSIS TODAY, vol. 159, no. 1, pp. 84-95, 2011. European Conference on Combinatorial Catalysis Research (EuroCombiCat2009), Inst Chem Technol, Gandia, SPAIN, MAR 26-29, 2009.

Research Report of the team in 2010—2014

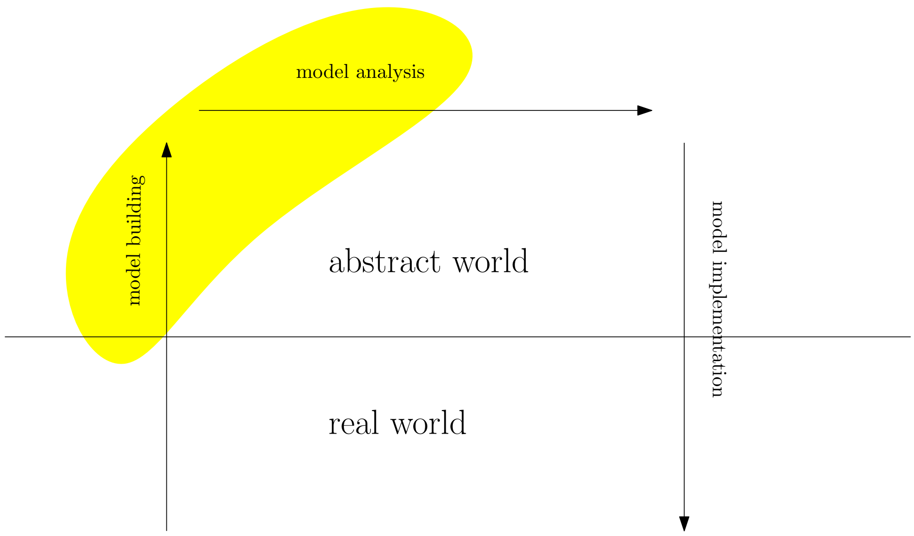
Institute	Institute of Computer Science

Scientific team	Optimization and Systems

2.1 Introduction: The Big Picture

The department constituting this team came into existence in July 2013, with members originating from several organizational units that had been in existence until that date. In this report we survey results from the whole period under evaluation. Those results have, to a large extent, been achieved already before the existence of the current department.

A fundamental ingredient of how science has influenced the modern world are models: abstract and general descriptions of reality, often formulated in the language of mathematics. Currently, such models are more and more penetrating industrial engineering practice, mainly due to the spreading of model based design. The work of the department can be described using the following figure illustrating how humans work with such models:



The starting point for our work is the automatization of the first two phases of this process: model building and model analysis. This usually proceeds by simplifying the original problem to simpler and more abstract problems, in our case usually problems of optimization and constraint solving, which are a main focus of our work:

Summing up, in our research in 2010—2014 we did

basic research on the automatization of
model building and analysis*,*
with a special focus on the underlying
optimization/constraint solving *techniques.*

In the rest of this document we will first (Sections 2.2 and 2.3) highlight examples of results in these directions, and will then (Section 2.4) give a more comprehensive overview of our work. The first highlight (Section 2.2) is an example of a result in the area of constraint solving, and the second highlight (Section 2.3) in the area of model analysis.

2.2 Highlight 1: Systems of Equations

One of the oldest and most important computational problems is solving systems of equations $f = 0$ with $f : \mathbb{R}^k \to \mathbb{R}^n$. Classical methods usually study the problem of iteratively improving numerical approximations of individual solutions. However, the problem of checking whether such a system of equations has a solution at all, is undecidable as soon as a periodic function symbol such as sin is allowed. We showed that by slightly modifying the problem, checking the existence of robust solutions (i.e., solutions that do not vanish under continuous perturbation of f) in a compact domain, the problem can be reduced to a classical problem from topology (extension of maps into a sphere), shedding new light onto decidability of the problem. The corresponding paper [2], originally published in the proceedings of the conference SODA was in the mean-while accepted for publication by the Journal of the ACM (collaboration with Marek Krčál, IST Austria).

2.3 Highlight 2: Quasi-decidability of Verification of Hybrid Dynamical System

A hybrid dynamical system is a dynamical system that has partially discrete, partially continuous state and evolution. Since computation is usually modeled using discrete models and physical processes using continuous models, hybrid dynamical systems are an important tool for modeling systems from the real world that integrate computation with physical processes (cf. the notion of cyber-physical system).

We studied the problem of formal safety verification of hybrid systems. This problem is undecidable, except for very special cases. In our result, we circumvent undecidability by providing a verification algorithm that provably terminates for all robust problem instances, but need not necessarily terminate for non-robust problem instances. A problem instance x is robust if and only if the given property holds not only for x itself, but also when x is perturbed a little bit. Since, in practice, well-designed systems are usually robust, this implies that the algorithm terminates for the cases occurring in practice.

The journal in which the paper [12] describing this result appeared, arguably is the leading journal in formal verification (e.g., it has the Turing award winners Edmund M. Clarke and E. Allen Emerson on its editorial board).

2.4 Overview of Research in 2010–2014

We will now survey our research in the evaluation period in more detail, structured according to the three areas identified in the introduction: model building (Section 2.4.1), model analysis (section 2.4.2), and optimization/constraint solving (Section 2.4.3). Throughout this section we only cite typical publications. The full list of publications is a separate deliverable of the evaluation exercise.

2.4.1 Model Building

- Meta-learning: Machine learning is a field that studies the automatic building of models of the real world. We did extensive work on meta-learning, that is, the application of machine learning techniques to improve the techniques of machine learning themselves, for example, automatically choosing an optimal machine learning method or some of its parameters for a certain application class. Here, we used our expertise in optimization, in this case evolutionary optimization algorithms [14].

- Cyber-physical systems architecture: Cyber-physical systems are systems that integrate computation and physical processes. We studied general principles of how to build reliable cyber-physical systems [1].

- Cell biology: We cooperated with biologists, using our expertise on numerical optimization to improve models of certain cells from experimental data [6].

2.4.2 Model Analysis

- Automatic computation of Lyapunov functions: The problem of proving stability of a given dynamical system and providing a corresponding basin of attraction has been studied since the 19th century, and has been in the center of the field of control theory since then. Still, for non-linear systems, such problems have to a large extent defied complete automatization. We published a paper that brings us significantly closer to the completely automatic solution of this problem [13] (collaboration with Zhikun She, now Beihang University, Beijing, China).

- Formal verification: In addition to the result highlighted in Section 2.3 we also published several further results on the formal verification of hybrid dynamical systems. For example, a method for safety verification of hybrid dynamical systems whose discrete dynamics also allows probabilities [17, 18] (collaboration with Universität Saarbrücken, Germany), or a method for reducing the problem of falsification (i.e., finding errors of incorrect systems) to classical numerical optimization problems [7].

2.4.3 Optimization and Constraint Solving

- A large part of our research has been devoted to numerical optimization. We concentrated especially on large-scale optimization (more than 1000 and typically 10000 variables): Classical numerical optimization techniques are, to a large extent, built on matrix operations. However, since the size of matrices grows quadratically with the problem dimension, this is not feasible for large optimization problems. In order to be able to handle such problems, one can use approximating vectors instead of matrices, exploit matrix sparsity etc., while at the same time ensuring efficient convergence of the resulting algorithms. We produced several results in this direction [8, 9, 15, 16], giving evidence for their practical efficiency based on implementations in our software package UFO (`http://www.cs.cas.cz/luksan/ufo.html`) that serves as a test-bed for all our algorithms in the area of numerical optimization.

- In addition to the result highlighted in Section 2.2 we produced several results in numerical constraint solving:

  For the automatic analysis of continuous models it is often useful to solve constraints with quantifier prefix $\exists\forall$. Here the existential quantifier ensures the existence of a certificate of a certain property that holds globally, as ensured by the universal quantifier [5] (collaboration with Milan Hladík, Charles University).

  We also proved an analoguous result to the highlight described in Section 2.3 for the solving of a certain class of constraints forming a fragment of the first-order theory of real numbers: the fragment is undecidable, but we proved it to be quasi-decidable [4] in a similar way as described in Section 2.3 (collaboration with Piotr Zgliczynski, Jagellonian University, Cracow, Poland). The main ingredient for the proof is the notion of topological degree, and we designed a new, and efficient algorithm for computing this degree [3].

- We did work on evolutionary optimization, that is, optimization techniques that are inspired by elements of biological evolution such as mutation or natural selection. Here we concentrated on problems of multi- and many-objective evolutionary optimization [10, 11].

Research Report of the team in the period 2010–2014

Institute	Institute of Computer Science of the Czech Academy of Sciences

Scientific team	Department of Fundamental Topics

The Department of Fundamental Topics was formed in the mid of 2013 during the reorganization of the Institute of Computer Science.

Highlights

G-matrices by Miroslav Fiedler

Professor Miroslav Fiedler was born in 1926. In his fields of interest, matrix theory, graph theory and their relationship with other parts of mathematics and applications, he published between 2010 and 2014 one book and about 20 research papers. As an invited speaker, he participated at more than 10 international meetings, he is a member of five editorial boards of international journals and his interests include also mathematical Olympiads for secondary school students. He has a fruitful collaboration with Frank Hall from Georgia State

University, Atlanta, USA, on topics in combinatorial matrix theory. In 2013, he was awarded the Hlávka medal (The prize named to honor Josef Hlávka, a Czech architect, building contractor, politician, and the largest Czech patron.) for all life achievements.

Particularly interesting is the paper [10] by M. Fiedler and F.J. Hall, where they define a new type of matrix called G-matrix. The G-matrix is a real nonsingular matrix having the property that the transpose of its inverse can be written as a multiple of the original matrix by nonsingular diagonal matrices from both sides. It is a real nonsingular matrix that has very general features. Among G-matrices belong many special matrices including all Cauchy matrices, orthogonal matrices, and nonsingular diagonal matrices. If a matrix is a G-matrix then also its inverse, its transpose, the product of the square G-matrix with nonsingular diagonal matrix, the product of the square G-matrix with a permutation matrix, and the direct sum of G-matrices are also G-matrices. There is also an important theorem that says that a 2×2 matrix is G-matrix if and only if it is nonsingular and has four or two nonzero entries as shown in examples.

Examples: G-matrices $\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix}, \begin{bmatrix} 0 & 2 \\ 3 & 0 \end{bmatrix}$

Not G-matrices: $\begin{bmatrix} 1 & 2 \\ 3 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 4 \end{bmatrix}$ (3 and 1 entry) or $\begin{bmatrix} 1 & 0 \\ 3 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 2 \\ 0 & 4 \end{bmatrix}, \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}$ (singular).

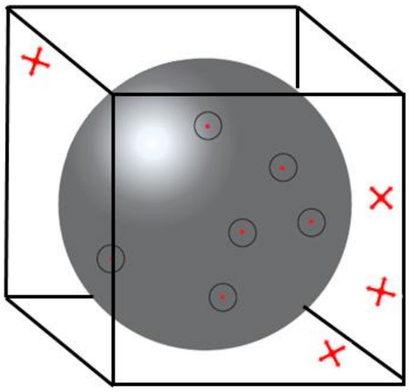
It is interesting to note that in the same year (2012) a first citation follows in the paper[1] by Masaya Matsuura where is given a generalization of G-matrices, the GG-matrices, so that one can deal with not only nonsingular matrices but also with square singular matrices and rectangular matrices.

Model complexities of feedforward networks by Věra Kůrková

The paper [2] presents a new methodology for estimation of the rate of convergence that is based on integral transforms with kernels induced by network units.

In more detail and from application point of view, V. Kůrková reduces complicated mathematical assumptions about characteristics of components of shallow neural networks (with one hidden layer) into very natural conditions and proves an estimate of the rate of approximation. The conditions mentioned include boundedness and finiteness that can be easily verified. From the estimate it follows that geometrical features of input data are important.

This result can be illustrated as follows. The probability that a randomly chosen function on $\{0; 1\}^d$ cannot be represented by a shallow perceptron network with the number of units and sizes of output weights depending on dimension d polynomially approaches certainty. It means that due to the geometry of high-dimensional spaces most functions on high-dimensional cubes cannot be tractably represented by shallow networks. On the other hand, functions in a d-dimensional sphere can be tractably represented by shallow networks. In this case the rate of approximation converges fast and high input space dimensionality does not matter.



[1] Matsuura, M: A note on generalized G-matrices. *Linear Algebra and its Applications*, Vol. 436 (2012) pp. 3475–3479.

Verification of Linear (In)Dependence in Finite Precision Arithmetic by Jiří Rohn

In his paper [3] J. Rohn deals with the problem of verification of linear dependence or independence of columns of a matrix by means of finite precision arithmetic. This means, given a matrix *A* where its entries are floating-point numbers on a given computer (with limited precision), we wish to decide whether *A* has linearly independent columns or *A* has linearly dependent columns or the problem is undecidable.

The result is

- Matrix *A* has linearly <u>independent</u> columns if
  $$\|I - RA\|_1 < 1$$
  where *R* = computed pseudoinverse matrix. (There exist tools for computing *R*.)
- Matrix A has linearly <u>dependent</u> columns if
  $$\boldsymbol{C} = I - \boldsymbol{B}A = [\underline{C}, \overline{C}]$$
  where *B* is verified enclosure of pseudoinverse of *A* and
  $\underline{C}_{ij} > 0$ or $\overline{C}_{ij} < 0$ for some *i, j*.
  (There exist tools for computing matrix *B* and also tools for computing interval matrix *C*.)
- Else there is <u>no verified result</u>.

The author characterizes this result: “While verification of linear independence poses no problem, verification of linear dependence is by no means easy. The clue to the solution of this problem consists in the use of a verified pseudoinverse which, in turn, requires use of a verified singular value decomposition. In the nutshell, the problem can be solved by finite precision means, but at the expense of employing heavy machinery.”

Topics

The team works on the following topics:

- Computational models with respect to complexity, computability and efficiency
- Neural networks with layered structure from the point of view of complexity estimates and speed of convergence
- Features and behavior of special kinds of matrices, their relation to graphs theory
- Interval computations, interval matrices, solution of special computational tasks of linear algebra
- Structure and behavior of uniform sequences
- Fractal nature of multidimensional data, hidden structures of high dimensional real and binary data, their influence on the behavior of clustering and kernel methods
- Robust estimations and robust regression with the use of scalar score functions
- Factor analysis, Boolean factor analysis, recurrent neural networks research
- Selected applications, especially in brain studies, human joints and landslides

Research output of the team

Computational models with respect to complexity, computability and efficiency

The research in this field can be characterized as a quest for understanding computation. In cooperation with Jan van Leeuwen *Jiří Wiedermann* developed a new, alternative definition of computation where computations are seen as observer-dependent knowledge generating processes [4]. Another result of J. Wiedermann is a progress in solving more than 40 years old conjecture by Hopcroft, Paul and Valiant from 1974 concerning the relation between nondeterministic time and nondeterministic space [5]. Two conference papers [6, 7] related to the problem of verification of matrix multiplication have attracted quite an interest since they present the first progress after 35 years since R. Freivalds has published his well-known probabilistic algorithm in 1979.

Neural networks with layered structure from the point of view of complexity estimates and speed of convergence

The research of *Věra Kůrková* was focused on mathematical theory of feedforward neural networks. Her results, e.g. [8, 9], provide a theoretical foundation for the field of research which mostly develops as an experimental discipline. The papers investigate capabilities and limitations of various types of neural networks to solve efficiently high-dimensional tasks. Papers also provide estimates of model complexities of networks in dependence on various types of computational units (perceptrons, radial, and kernel units), size and type of training data, and their dimension. She developed a new method, which is based on integral transformations in the form of networks with continua of computational units. The method was applied to non-traditional solutions of Fredholm integral equations exploiting approximate solutions computable by neural networks.

Features and behavior of special kinds of matrices, their relation to the theory of graphs

One of the most important team output published in the last five years is the book "Matrices and Graphs in Geometry" (Cambridge University Press, 2011) by *Miroslav Fiedler*. The book acquaints the reader with basic matrix theory, graph theory and elementary Euclidean geometry so that one can appreciate the underlying connections between these various areas of mathematics and computer science. Simplex geometry is a topic generalizing geometry of the triangle and tetrahedron. The appropriate tool for its study is matrix theory, but applications usually involve solving huge systems of linear equations or eigenvalue problems, and geometry can help in visualizing the behavior of the problem. In many cases, solving such systems may depend more on the distribution of non-zero coefficients than on their values, so graph theory is also useful.

Interval computations, interval matrices

The results of *Jiří Rohn* can be grouped into two categories. First, linear problems with inexact data; second, theory and algorithms for solving equations and inequalities involving absolute values. In the first category, the main result [22] is an algorithm for solving systems of interval linear equations. In the second category, he found, for example, an algorithm for finding all solutions of the equation $Ax+B|x|=b$ [12]. These results have been published as 15 papers in impacted journals and technical details including programs are subject of 45 research reports. Programs included in reports together with examples make deep and difficult problems that were thoroughly mathematically solved, accessible for practical computations.

Structure and behavior of uniform sequences

Štefan Porubský investigated arithmetical properties of number sequences, especially behavior of fractional parts of irrational multiples of positive integers within unit interval. The most important result is his book about uniform sequences [13]. Authors generalized known results and also discovered new aspects of distributional properties. Some of them have impact on the pseudorandom generators and applications in quasi Monte Carlo methods. They defined a new type of topology and density concept, which implies infiniteness in generalized arithmetic progressions. As a byproduct new proofs of the infinitude of prime numbers were obtained [14].

Fractal nature of multidimensional data, hidden structures of high dimensional real and binary data, their influence on behavior of clustering and kernel methods

Marcel Jiřina in [15, 16] used notion of the distribution mapping function that maps the layout of points in neighborhood of a fixed point. Thus he transformed a multidimensional space on a one dimensional space of distances from the fixed point. He also found that the famous correlation integral according to Grassberger and Procaccia can be decomposed into a set of distribution mapping functions. Moreover he has shown that the distribution mapping function can be approximated by a polynomial function with an exponent called a distribution-mapping exponent. This finding he used for constructing new classifiers that use rather strange kernels that do not conform standard Mercer's conditions to be finite and have finite integral.

Robust estimations and robust regression with the use of scalar score functions

Zdeněk Fabián developed the "score function of distribution" [17]. The function generalizes the concept of the likelihood score of parametric distributions. In some ‚favorable' cases it equals to the classical likelihood score for a parameter expressing the ‚center' of the distribution. He has shown that to any regular continuous distribution function can be assigned the score function of distribution by a unique way. The score function of distribution appears to be a suitable tool for the description, study and comparison of models of continuous random variables [18].

Factor analysis, Boolean factor analysis, and recurrent neural networks research

The research of *Dušan Húsek* and his colleagues was focused on developing and analyzing new architectures of neural networks with application to data analysis and machine learning methods with application in the brain computer interface. The main research result in binary recurrent neural networks research was a discovery of a new neural network based on associative memory and able of generalization rather than finding of missing parts of information only [19]. For dimensionality reduction of binary data there were developed and published four algorithms, two methods of neural network-based binary factor analysis, and two model-based statistical algorithms, e.g. [20].

Selected application in brain studies, human joints and landslides

D. Húsek performed brain studies within the frame of the brain computer interface. Activities of *Jiří Nedoma* in the period 2010-2014 included constructions of mathematical models of the biomechanics of the human skeleton and its parts. In 2011 he published the book *Mathematical and Computational Methods in Biomechanics of Human Skeletal Systems. An Introduction* [21].

Quality and scientific relevance

During the period 2010-2014 the researchers in department 27 produced 281 results of different kind. A summary can be found in the Table below at the left hand side. In the Table at the right hand side citations according to WOS and Scopus databases are shown. It includes the lifetime citations in the upper part and citations obtained during the years 2010 till 2014 in the bottom part. The abbreviation “AC” means autocitations.

Publication	Amount
Book – monograph	3
Book Chapter	20
Journal impact	53
Journal other	30
Conference proceedings	4
Foreign conference paper	68
Home conference paper	8
Software	2
Utility model	1
Report	72
Abstract	20
Total	281

Parameter	Amount
Team H-index	27
Citations WOS	4504
Citations Scopus	3453
Citations WOS without AC	3795
Citations Scopus without AC	2665
2010-14: Citations WOS	216
2010-14: Citations Scopus	1460
2010-14: Citations WOS without AC	147
2010-14: Citat. Scopus without AC	1090

Earning capacity

In 2010 – 2014 there were 13 projects granted either by the Czech Ministry of Education (MED) or by the Grant Agency of the Czech Academy of Sciences (CAS). They brought a total of 970 000 Euro. These projects are listed in Table below and include projects of main investigators from the team. Team members in projects of other teams are not listed.

Name of the project	**Supported by**	**Amount (1000 Euro)**	**Main investigator**	**From**	**To**
Methods of artificial Inteligence in GIS	CAS	25	Húsek	2009	2011
Decompositions of matrices with binary and ordinal data: theory, algorithms, and complexity	CAS	42	Húsek	2010	2012
Centre for applied cybernetics	MED	372	Jiřina	2005	2011
Complexity of perceptron and kernel networks	CAS	20	Kůrková	2008	2010
Model complexity of large fuzzy rule-based systems and neural networks	MED	2	Kůrková	2009	2010
Analysis of intelligent computational distributed systems	MED	60	Kůrková	2010	2012
Aproximation and learning of multivariable functions by neural networks	MED	22	Kůrková	2010	2012

Name of the project	Supported by	Amount (1000 Euro)	Main investigator	From	To
Learning of functional relationships from high-dimensional data	CAS	171	Kůrková	2011	2013
Modeling of complex systems by soft-computing methods	MED	25	Kůrková	2013	2016
Analysis of intelligent distributed computational models	MED	108	Kůrková	2010	2012
Aproximation and learning of fuctions with many variables using neural networks	MED	21	Kůrková, Neruda	2010	2012
Number theory and its applications	MED	1	Porubský	2012	2013
Distribution and metric properties of number sequences and their applications	CAS	76	Porubský	2012	2015
Number theory and its applications	MED	0	Porubský	2014	2015
Res informatica	CAS	24	Wiedermann	2009	2012

13 projects	**TOTAL**	**970**	**5 researchers**

Cooperations

In the Table below are summarized cooperations that resulted in a publication.
It can be found out that majority of coauthors of team members are from abroad.

Team member	Coauthor	Institute	Theme
Rohn	Farhadsefat, R.	Faculty of Basis Sciences, Hamadan Branch, Islamic Azad University, Hamadan, Iran	Interval matrices
	Hooshyarbakhsh, V., Lotfi, T.	Department of Applied Mathematics and Computer Sciences, Hamedan Branch, Islamic Azad University, Hamedan, Iran	Interval matrices
Fiedler	F. Hall	Georgia State University, Atlanta, USA	Combinatorial matrix theory
Kůrková	Kainen,P.C. - Vogt, Andrew	Georgetown University, USA	Shallow neural networks and integral transforms.
	Sanguineti, M.	University of Genova, Italy	Shallow neural networks and integral transforms.
	Gnecco, G	IMT Institute for Advanced Studies Lucca, Italy	Shallow neural networks and integral transforms.

Team member	**Coauthor**	**Institute**	**Theme**
Húsek	Řezanková, H.	ICS	Brain computer inteface.
	Frolov, A.I. Polyakov, P.Y.	Institute of Higher Nervous Activity and Neurophysiology, Russian Academy of Sciences, Moscow	Boolean Factor Analysis, Brain computer inteface.
	Snášel, V.	TU (VSB) Ostrava	Brain computer inteface.
	Mokienko, O. - Bobrov, P. - Chernikova, L. - Konovalov, R.	Nauchny Center of Neurology, Moscow OR Rossiysky National Research Medical University. NI Pirogov, Moscow	Brain computer inteface.
	Gucek, D.	Institute of Information Theory and Automation CAS	Brain computer inteface.
Fabián	Jiřina, M.	ICS	Score linear regression
	Jordanova, P.	Faculty of Mathematics and Informatics, Shumen University, Shumen, Bulgaria	Score approaches to testing for normality and for fitting heavy-tailed distributions
	Stehlík, M. - Waldl, H.	Department of Applied Statistics, Johannes Kepler University in Linz, Linz, Austria	Score approaches to testing for normality and for fitting heavy-tailed distributions
	Střelec, L.	Department of Statistics and Operational Analysis (FBE), Mendel University, Brno, Czech Republic.	Score approaches to testing for normality and for fitting heavy-tailed distributions
	Potocký, R.	Department of Mathematics and Statistics, Comenius University, Bratislava	Score approaches to testing for normality and for fitting heavy-tailed distributions
Wiedermann	Jan van Leeuwen	Department of Computer Science, Utrecht University	Computational power of unbounded processes
	Petrů, L.	Faculty of Mathematics and Physuics, Charles University in Prague	Computational power of unbounded processes
Jiřina	Fabián, Z.	ICS	Score linear regression
	Jiřina, M. ,jr.	Faculty of Informatics, Czech Technical University in Prague.	Scaling in distance-based classifiers.
Nedoma	Daněk, J.	ICS	Contact tasks, partial differential equations, finite elements method. Human joints, landslides.
	Mahdian, N. Dostálová, T. Kohout, J. Hubáček, M. Hliňáková, P.	Charles University, 2nd Medical Faculty, Department of Paediatric Stomatology, University, Hospital in Motol, Prague, Czech Republic	Contact tasks, partial differential equations, finite elements method. Stomatology.
Porubský	Besser, B.P.	Österreichische Akademie der Wissenschaften, Institut für Weltraumforschung, Graz, Austria	Paper "Jakob Philipp Kulik and his work in Graz"
	Marko, F.	Pennsylvania State University, Hazleton, USA	Density and the Dirichlet Condition.
	Strauch, O.	Matematical Institute, Slovak Academy of Sciences, Bratislava	Book
	Grošek, O.	Institute of Computer Science and Mathematics, Slovak University of Technology, Bratislava	Coprime solutions to $ax = b$ (mod n).

Team member	Coauthor	Institute	Theme
Daněk, J.	Nedoma, J.	ICS	Contact tasks, partial differential equations, finite elements method. Human joints, landslides.
Řezanková, H.	Húsek, D.	ICS	Brain computer inteface.

Selected publications cited above

[1] Fiedler, M.: *Matrices and Graphs in Geometry*, Cambridge: Cambridge University Press, 2011.

[2] Kůrková, V: Complexity estimates based on integral transforms induced by computational units. *Neural Networks*, Vol. 33, September 2012, pp. 160-167.

[3] Rohn, Jiří: Verification of Linear (In)Dependence in Finite Precision Arithmetic. *Mathematics in Computer Science* Vol. 8, No. 3-4 (2014), pp. 323-328.

[4] Wiedermann, J. - van Leeuwen, J.: Computation as Knowledge Generation, with Application to the Observer-Relativity Problem. *Proceedings of the 7th AISB Symposium on Computing and Philosophy, 2014* - (Ed.: Erden, Y.), pp. 1-8. [AISB Symposium on Computing and Philosophy /7/. Goldsmiths (GB), 01.04.2014-04.04.2014]

[5] Wiedermann, J.: Complexity of Nondeterministic Multitape Computations Based on Crossing Sequences. In: *Description Complexity of Formal Systems.* (Ed.: Holzer, M.; Kutrib, M.; Pighizzini, G.) - Berlin: Springer, 2011, pp. 314-327 (ISBN 978-3-642-22599-4, ISSN 0302-9743) Held: DCFS 2011. International Workshop on Descriptional Complexity of Formal Systems /13/. (Lecture Notes in Computer Science. 6808)

[6] Korec, I. - Wiedermann, J: Deterministic Verification of Integer Matrix Multiplication in Quadratic Time. In: SOFSEM 2014. *Theory and Practice of Computer Science*. Cham: Springer, 2014 - (Eds.: Geffert, V. - Preneel, B. - Rovan, B. - Štuller, J. - Tjoa, A.), pp. 375-382 ISBN 978-3-319-04297-8. ISSN 0302-9743. - (Lecture Notes in Computer Science. 8327).

[7] Wiedermann, J.: Fast nondeterministic matrix multiplication via derandomization of Freivalds' algorithm. In: J. Diaz - I. Lanese - D. Sangiorgi (Eds.): *Theoretical Computer Science - 8th IFIP TC 1/WG 2.2 International Conference, TCS 2014*, Rome, Italy, September 1-3, 2014. Proceedings, Lecture Notes in Computer Science, Vol. 8705, Springer, pp. 123-135, 2014.

[8] Gnecco, G. - Kůrková, V. – Sanguineti, M.: Some comparisons of complexity in dictionary-based and linear computational models. *Neural Networks*, Vol. 24, No. 2, pp.171-182, 2011.

[9] Kůrková, V. - Kainen, P. C.: Comparing fixed and variable-width Gaussian networks. *Neural Networks*, Vol. 57, pp. 23–28, 2014.

[10] Fiedler, M. - Hall, F. J.: G-matrices. *Linear Algebra and Its Applications*. Vol. 436, No. 3 pp. 731-741, 2012.

[11] Fiedler, M. - Markham, T. L.: More on G-matrices. *Linear Algebra and Its Applications*. Vol. 438, No. 1, pp. 231-241, 2013.

[12] Rohn, Jiří: An algorithm for computing all solutions of an absolute value equation. *Optimization Letters*. Vol. 6, No. 5, pp. 851-856. ISSN 1862-4472, 2012.

[13] Strauch, O. - Porubský, Š.: *Distribution of Sequences: A Sampler* (First electronic revised and extended edition, December 11, 2013). 651 pages. Available at: https://math.boku.ac.at/udt/books/MYBASISNew.pdf

[14] Grošek, O. - Porubský, Š: Coprime solutions to ax = b (mod n). *Journal of Mathematical Cryptology*, Vol. 7, No. 3, pp. 217-224. ISSN 1862-2984, 2013.

[15] Jiřina, M. - Jiřina jr., M.: Correlation Dimension-Based Classifier. *IEEE Transactions on Cybernetics*, Vol. 44, No. 12, pp. 2253-2263. ISSN 2168-2267, 2014.

[16] Jiřina, M. - Jiřina jr., M.: Utilization of Singularity Exponent in Nearest Neighbor Based Classifier. *Journal of Classification*, Vol. 30, No. 1, pp. 3-29. ISSN 0176-4268, 2013.

[17] Fabián, Z.: A New Statistical Tool: Scalar Score Function. *Computer Technology and Application*, Vol. 2, pp. 109-116. ISSN 1934-7332, 2011.
[18] Fabián, Z.: Score Function of Distribution and Heavy-tails. *Proceedings of COMPSTAT 2014. Geneva*: Centre international de conferences, 2014 - (Gilli, M. - Nieto-Reyes, A. - González-Rodríguez, G.), pp. 657-664 ISBN 978-2-8399-1347-8.
[19] Frolov, A. A. - Húsek, D. - Muraviev, I. P. - Polyakov, P.Y.: Origin and Elimination of Two Global Spurious Attractors in Hopfield-Like Neural Network Performing Boolean Factor Analysis. *Neurocomputing,* Vol. 73, 7-9, pp. 1394-1404. ISSN 0925-2312, 2010
[20] Frolov, A. A. - Húsek, D. - Polyakov, P. Y.: New BFA Method Based on Attractor Neural Network and Likelihood Maximization. *Neurocomputing,* Vol. 132, 20 May 2014, pp. 14-29. ISSN 0925-2312
[21] Nedoma, J. - Stehlík, J. - Hlaváček, I. - Daněk, J. - Dostálová, T. - Přečková, P.: *Mathematical and Computational Methods in Biomechanics of Human Skeletal Systems. An Introduction.* Wiley Series in Bioinformatics, 2011.
[22] Rohn, J.: An algorithm for computing the hull of the solution set of interval linear equations. *Linear Algebra and Its Applications*. Vol. 435, No. 2, pp. 193-201. ISSN 0024-3795, 2011.