

# **Evaluation of the Research and Professional Activity of the Institutes of the Czech Academy of Sciences (CAS) for the period 2010–2014**

## **Final Report on the Evaluation of the Institute**

**Name of the Institute:** Institute of Computer Science of the CAS, v. v. i.

**Fields, in which the Institute registered its teams:**

Mathematics

Observer representing the Academy Council of the CAS: Michal Haindl

Observer representing the Institute: Julius Štuller

Substitute observer: Dr. Duintjer Tebbens

**Commission No. 1: Mathematics**

Chair: Professor Willi Jäger

Date of the visit of the Institute: December 2, 2015

Program of the visit of the Institute: see attached Minutes from the visit

Evaluated research teams:

*No. 1 - Department of Computational Methods*

## **A. Evaluation of the Institute as a whole**

### Remark:

*The Commission Mathematics has to evaluate only 1 team of the Institute. It is not able to evaluate the Institute as whole correctly, due to lacking information.*

*Whereas in case of other Institutes, the general written and the oral report of the Institute gave a survey on the scientific program and achievements of all departments, allowing some comments, this is not the case for this Institute.*

## **1. Introduction**

The Institute started 40 years ago as a computing center, later on one of its parts was transformed into a research institute. The Institute reported a substantial restructuring of this research institute in 2013. However, its history left traces, which are still visible in the current structure. The guidelines of the restructuring seem not to be set according to clearly formulated scientific visions. They may have followed current needs of the management. There are no clear rules visible, used in allocating scientific

areas to canonic disciplines. However, the division has not only administrative but also scientific consequences. Decompositions of units in subunits are finally structural decisions, determining a “topology” influencing the future development.

The following Departments were finally established, partially based on already existing and successfully working teams:

*The Department 1 “Computational Methods”*

is the only department allocated officially to the Commission Mathematics. This is a correct decision, since its research field belongs mainly to Numerical Linear Algebra, an important sub-discipline of Numerical Mathematics. The report of this department provides clear information needed for an evaluation, in particular of the scientific potential, the performance and its impact.

In the following we try to sketch the character of the other Departments, which the report of Institute should have been introduced more precisely. Thus, we intend to describe the structure of the Institute, information needed to make some comments from our point of view, which admittedly is restricted.

*Department 2 “Theoretical Computer Science “*

is focused on Computational Complexity and those sub-disciplines of Mathematical Logics connected with this topic. CAS shares with all Universities, which have Logic as discipline, the problem, whether to allocate it to Mathematics, to Computer Science or to Philosophy. Just splitting disciplines into sub-disciplines is endangering the substance of the discipline as whole. Complexity Theory and Fuzzy Logics are perfect examples, where the allocation even for sub-disciplines is multivalued.

*Department 3 “Nonlinear Modeling“*

has a rather general title, not really representing „Environmental Informatics“, mentioned as its main field of interest. The presented information does not allow to identify, where the research is located: in modeling, in simulation, in data processing, in data analysis, ... , and in what area which specific contributions can be reported.

*Department 4 “Medical Informatics and Biostatistics”*

Is dedicated to Biostatistics and Reduction of Complexity in high dimensional data, their applications lie in Life Sciences and in particular in Genetics. Especially in medical applications the number of data variables may be large, and the sample numbers very small. This a very typical situation in reality, requiring methods different from statistical methods used in more standard situations.

*Department 5 “Nonlinear Dynamics and Complex Systems”*

is also involved in processing of high dimensional data and in data mining, in developing and applying methods enabling to discover causal relations in time series analysis. The developed methods are applied to electrophysiological data from neurosciences and from multi-scale atmospheric dynamics.

*Department 6 “Optimization and Systems“*

The scientific topic and the structure of this department are left totally unclear. This fact is another example, where the report of the Institute does not fulfill the requirements. The mere reference alone to the individual reports of the Department is not sufficient, and of no use, if there is no direct access to their files.

*Department 7 Fundamental Topics*

This Department „consists mostly of scientific personalities studying diverse topics which could be interesting for other groups in the institute.“(Report of the Institute) This construct may have its charm, but it is not clear it really fulfills the expectations.

In the present situation, the Commission just summarizes its observations and comments in only in one section, instead of a section “Strengths “ and a section “Weaknesses”, which both require more knowledge about the scientific structure, performance and future plans of the individual departments. Thus, we try to avoid statements, leading to disadvantages for a department due to incomplete information.

## **2. Comments to the situation of the Institute**

The Commission awards a top grade to Department 1 “Computational Methods”. The Panel II evaluation is in agreement with the following result of the evaluation of the outputs evaluated in Panel I:

30 % „world leading“, 60 % „internationally excellent“, 10 % „recognized internationally“

An indicator for the scientific quality of the Departments in average is the following result of the Institute as whole:

14 % „world leading“, 38 % „internationally excellent“, 38 % „recognized internationally“.

9 % „recognized nationally“ 1% „ below recognized nationally“

A focused scientific profile is described for Department 1- 5. The Departments 4,5 and as it appears also 3 are concentrated on the processing and mainly statistical analysis of large data sets. They are strongly oriented to applications. The required methods of Statistics are crucial tools and cannot be taken from the shelf, due to the character of the data sets, arising e.g. in environmental or medical problems.

The Institute of Computer Sciences is representing a spectrum of research areas, which is only partially in the core of Computer Sciences. Some of the missing ones exist in the Institute of Information Theory and Automation.

Here the question arises, where the basic research in Statistics necessary for application oriented research is located and where it should be located in CAS. The same questions arise for other research fields like Numerical Mathematics, Computational Sciences, Data Mining or Machine Learning.

Not only the Commission but also several members of the CAS institutes are concerned about the fragmentation in the scientific structures and the programs. Even allocating excellent scientists to one unit does not guarantee that this unit is going to become and stay excellent. Sufficient evidence of scientific added value is required for the Departments 6 and 7.

The Commission is regretting not to be able to assist in this matter.

The report of the Institute has formulated not very significantly the future scientific program of the Institute, which should be its ID-card. Here again, the formulations in the Department reports may answer the remaining open questions.

A better coordination within the Academy, in particular with the Institute for Information Theory and Application, is required, but not in the field of view of the report of the Institute.

## **3. Recommendations**

The evaluation results of the Commission Computer Science, mainly responsible for most departments,

will strongly influence the decision, what measures have to be taken for the future development of the Institute.

Following the comments formulated above, Commission Mathematics recommends

- to give first priority to scientific concepts, based on a more careful analysis of the challenges and requirements in basic and application oriented sciences,
- to improve the cooperation of departments and institutes of CAS and Universities, in order to improve the coordination of research and education, to avoid fragmenting and duplicating, to support integrating and complementing activities,
- to strengthen the basic research in particular in statistics of large data sets,
- to strengthen respectively establish joint activities within the Nečas Center and a network in Computational Sciences and High Performance Scientific Computing.

It is necessary to ensure that institutes of CAS are not becoming a kind of scientific supermarkets, offering a broad mix of scientific products, also of medium quality and depending too much on the demand of customers.

## **B. Evaluation of the individual team**

### **Evaluation of the Team No. 1**

#### **Department of Computational Methods**

##### **1. Introduction**

This department is allocated to a Computer Science Institute, however, due to its orientation in research, it is even more appropriate to allocate it to computational mathematics. The focus of research is numerical linear algebra, dealing mainly with matrix computations. These are in general the final step in computing solutions to systems of equations.

The scientific program covers the following sub-topics

- 1) Iterative methods and sparse direct solvers for linear algebraic systems
- 2) Methods of preconditioning
- 3) Least square problems
- 4) Eigenvalue problems.

##### **2. Strengths and Opportunities**

These team and its achievements are an advertisement for numerical and computational research in CAS and in the whole Czech Republic. It is nationally and internationally linked to the best teams in Numerical Mathematics, representing strongly the algorithmic approach and building bridges to Computer Science and several areas of applications.

This kind of research is in great demand, since the development of computational methods, based on mathematical concepts and using algorithms, analyzed and optimized with mathematical tools, is as important for the progress in computing as the development computer-systems with computing-, communication- and storage-subunits, based on top technology and IT-concepts.

The team has made substantial contributions, documented very well also in top journals.

Ideas and methods, developed in this team provide also keys for reducing the complexity of systems, a very important topic of ongoing research. The availability of massively parallel computer with effi-

cient processors and units of processors, connected in networks with controllable topologies. Is going to affect the research in this team. Substantial impact on and contributions of this team to HPSC are to be expected. The team also has the potential to promote Numerical Analysis and to integrate existing teams in this field in a network, improving research and education. Several of its members are well imbedded in the Faculty of Mathematics and Physics of Charles University and the Nečas Center for Mathematical Modeling. This strong connection is very important for strengthening research and improving education in particular of PhD students.

### **3. Weaknesses and Threats**

The Commission does not see deficits, which are specific just for this team and are worth mentioning. However the team has like other teams the problem that the conditions, which can be offered to candidates for open positions, are not good enough; the resources are too limited and too unstable, to start new directions with new members.

There are not enough connections between the teams of CAS involved with numerical methods. The team is aware of this fact and is intended to support changes.

### **4. Recommendations**

The Commission recommends

- to increase the resources for the team to strengthen its research, e.g. in HPSC and Computational Sciences, in particular in systems reduction,
- to improve the cooperation of teams in CAS based on Numerical Mathematics,
- to strengthen the joint activities of Nečas Center,
- to establish a school for PhD students, a national network in High Performance Computing and Computational Sciences.

### **5. Detailed evaluations**

#### *Declaration on the quality of the results and share in their acquisition*

This team is internationally at the forefront of the Numerical Linear Algebra, which basic sub-discipline of Numerical Analysis, highly important for developing computational methods for complex systems.

The team has top expertise in Krylov subspace methods and iterative solution techniques. Its contributions to the developing and implementing new algorithms and to the analysis of their stability are most important. They have a great impact on numerical approximations of solutions to complex systems of equations, e.g. of model equations for real life processes.

The publication record is convincing, both with respect to quantity and quality. The Phase I evaluation rated the submitted outputs as follows,

30 % „world leading“, 60 % „internationally excellent“, 10 % „recognized internationally“.

#### *Declaration on the involvement of students in research*

The supervision of students is exceptionally positive. The question arises, why the situation differs from many other teams. One factor is surely the strong engagement of the team in teaching and the fact that leading scientists are members are also members of the university faculty, providing better access to students. Several advanced students were directly involved in research projects and publications of their results.

#### Declaration on societal relevance

The research program and the results obtained so far are highly important for Computational Sciences and their applications to a still growing number of human activities, where mathematical modeling, data based simulations and optimization and the use of state-of-the-art computer technology can find solutions to challenging problems.

Several members of the department are strongly involved in promoting Mathematics and the Sciences on national and international level in leading positions.

The team is focused on basic research, and is not directly involved in funded transfer projects.

#### Declaration on the position in the international and national context

The department is a prominent research team, imbedded in an international network of experts and partner teams mainly focused on numerical linear algebra, however also developing the available potential e.g. to complexity reduction and determining methods to project systems to adapted subspaces of the state space. The team has the experience and knowledge necessary to engage in High-Performance-Scientific-Computing (HPSC) both at national and international level. It is already a strong component of Nečas Center for Mathematical Modeling, which could be a central node also in a Czech network in Computational Sciences including the research part of HPSC. The numerical teams at the CAS and the Universities in Prague could form a strong numerical unit under the umbrella of the Center.

#### Declaration on the vitality and sustainability

The profile of the team in age and scientific activities seems to be quite balanced. For the future development a structured and properly funded, joint PhD-program of e.g. Charles University and CAS would be an excellent opportunity and support for the young generation. The fact that leading scientists of the Department are already members of both institutions is supporting further co-operation in particular in education and research in particular of PhD students.

#### Declaration on the strategy and plans for the future

The Department follows in its research strategy the research concepts of its leading scientists, what has proven to be quite successful in basic research, if the leaders are top scientists with visions. The topics of the running program are providing enough unsolved challenges. The intention to emphasize specific application areas, where the new methods developed in numerical linear algebra will be decisive solution tools, is strongly to be welcomed. System reduction is one of these methods, which have to be applied and tested in real life complex systems, which usually are nonlinear in its original form. To achieve the desired aims there has to be a better linking to algorithms designed for nonlinear systems.

There is a need for cooperation with the Department Numerical Analysis at the Institute of Mathematics of CAS. The interdisciplinary activities of the team within the Nečas Center in mathematical modeling, in High-Performance-Scientific-Computing and Computational Sciences in close co-operation with teams in Ostrava, in particular at the Supercomputing Center deserve strong support.

**Date:** February 14, 2016

**Commission Chair:** Professor Willi Jäger