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 Geonics 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: Josef Foldyna

Commission No. 1: Mathematics
Chair: Professor Willi Jäger

Date(s) of the visit of the Institute: Dec. 1, 2015
Programme of the visit of the Institute: see attached Minutes from the visit

Evaluated research teams:
No. 6 - Department of applied mathematics and computer science and IT4Innovations

Remark:
Several of the statements, the Commission has to make, apply also to other Institutes and the teams, which had to be evaluated. The Commission decided to formulate them more in detail and to send them in a letter to the President of CAS and the Chair of the Coordination Board of the Evaluation. We are going to refer to them by S and their number, as listed in the letter.
The Commission Mathematics has to evaluate only 1 team of the Institute. It is not able to evaluate the Institute as whole, due the obvious lacking information, however it is trying to make some comments, just from the perspective of the evaluated team. (S9)

A. Evaluation of the Institute as a whole

1. Introduction

The Institute has set up and supports the following teams engaged in basic research and applications in Geo- and Environmental Sciences. Engineering and Social Science:

1. Geomaterials,
2. Geomechanics,
3. Physical Geography,
4. Material Disintegration,
5. Human Geography,
6. Applied Mathematics
   (Department of Applied Mathematics and Computer Science and IT4Innovations).

Please note that the Institute defines its subunits in two ways: teams and departments. Here we use the team version.

The names of the institute and listed teams illustrate also the orientation of Team 6, which had to be evaluated by this Commission. The program of the Institute covers e.g.

- technologies for the utilization of the earth crust: mining, geothermal energy,
- technologies for solving environmental problems:
  management of waste, in particular of nuclear waste, CO_2 sequestration,
- modeling and simulation of geomechanical systems,
- analysis of physical and chemical properties of geomaterials,
- investigations of material disintegration.

Team 6 is providing the expertise and the tools in mathematical modeling, in developing numerical and computational methods to calibrate, simulate and validate model systems, to optimize the design of experiments, of technologies and engineering.
The establishment of the National Supercomputing Center (NSC), located in Ostrava, and the installation of a very powerful infrastructure for High-Performance Computing (HPC) are important steps forward into a future that will be even more influenced by Information Technology. The sciences will not just be important users of the massive parallel supercomputers, but will have a strong influence on IT, in particular through Mathematics and Computer Sciences. These disciplines play a basic role providing tools, simply subsumed under the term "software ", however necessary to make proper use of the hardware. To stress this fact, HPC is often replaced by HPSC, where S is an abbreviation of "scientific."
The Institute of Geonics and in particular its Team Applied Mathematics, Computer Science and IT4Innovations are challenged by the establishment of the NSC. They are already represented in the research program of the Supercomputing Center through the project "*Numerical Modeling for Engineering*".

2. Strengths and Opportunities

The expertise to solve the problems arising in the research areas of the Institute ranges from theory in mathematics and computer science to experiments in geosciences and material sciences. Multi- and cross-disciplinary activities and experience are distinguishing features of this Institute. It is strongly involved in project-oriented research on topics of high relevance for society.
E.g. research on geological deposition of waste, in particular of nuclear waste is extremely important, since it addresses a crucial problem of energy production and of protection of environment. The same holds true for research on CO_2 sequestering, an approach to control CO_2 as a factor in climate change.
The Commission has not received enough detailed information and only limited expertise to evaluate possible achievements of the Institute in these topics so far.
Having studied in detail the material of the Team *Applied Mathematics and Computer Science and IT24Innovation*, we only can state that there is sufficient expertise and scientific quality in mathematic modeling and computational methods, needed to contribute to research on these problem areas.
The Institute seems to be equipped quite well with laboratories providing experimental data needed for modeling and simulation, in particular for identification of system parameters and in some cases also for validation of model equations. This is an advantage, which has to be appreciated very highly.
The integration of several teams in the Supercomputing Center will open up enormous perspectives for simulation of the complex model systems arising e.g. in geophysics, material sciences and environmental sciences.
There is an urgent need to build up a network in Computational Sciences, at first on the national level. The human resources and the expertise of all competent teams in the country are needed. The Institute together with the National Center for Supercomputing can be the best catalysts in establishing such a network.

3. Weaknesses and Threats

The commission observes that the scientific quality in the Institute is varying. A factor might be that criteria for evaluating quality may vary. Whereas in mathematics publications are taken as main indicators of quality, this is no longer true for more experimental disciplines. Nevertheless, improving the scientific quality in the whole seems possible and is also advised.
New scientific challenging problems were identified, however, a more precise formulation of projects to solve them was missing in the reports. For example research on exploitation of geothermal energy is mentioned as one of possible future projects, without at least sketching an approach to this problem area and the available expertise, to overcome the difficulties arising in this kind of energy production.
The connections of the teams to the best research groups in the covered research area at least in Europe should be strengthened.
The problem how to attract young talents to join the research projects of the Institute remains unsolved, despite several efforts made by the Institute.
The Institute is strongly depending on third party money. This fact is creating instabilities for the financial as well as the human resources. On the other hand, cooperation with industry and other partners is providing information and chances for advances in research, which could not be obtained otherwise. Therefore it is important that a proper balance is achieved.

4. Recommendations

Based on the information available at present, the Commission recommends

- to intensify search for top scientists, preferable junior scientists, with the aim to form teams in new research areas,
- to take a more systematic approach to build up contacts to international leading teams in particular in computational sciences, geosciences, material sciences and high performance computing,
- to initiate in cooperation with the existing partners a national network in Computational Science, which finally should be integrated in an international network,
- to focus the future scientific program, giving priority to main challenges, identified by the Institute, and to promoting of HPSC.

Although it was not the main focus of the Commission, we also recommend strengthening the ties between the headquarters of the Institute with its branch in Brno.

5. Detailed evaluations

Due to the lack of more detailed information and the missing competence in most of the areas covered by the other teams, the Commission gives a detailed evaluation only for Team 6 in Part B. Under this heading, the Commission is only quoting the result of the Panel I evaluation of the outputs for Institute as whole

2% *„world leading“*, 16 % *„internationally excellent“*, 56 % *„recognized internationally“,*
25% *„recognized nationally“* 1% *„below the standard of nationally recognized“*

showing a shift compared to the performance of Team 6, a fact that was already mentioned in (3). To compare, the results just of Team 6 are quoted next:

7 % *„world leading“*, 36 % *„internationally excellent“*, 50 % *„recognized internationally“,*
7 % *„recognized nationally“*.

The obvious shift in the rating was already mentioned and commented before.

B. Evaluation of the individual team

Evaluation of the Team No. 6

Department of Applied Mathematics and Computer Science and IT4Innovations

1. Introduction

This team is integrating in its program Mathematical Modeling, Simulation and Optimization (MOS), a research field combining Mathematics, Computer Science and application disciplines. Due to the long tradition of the Ostrava region in mining and heavy industry, the Geosciences, Environmental Sciences and Engineering Sciences are in the focus of applications. The establishment of the National Center for Supercomputing in Ostrava has already had an important impact on the regional and national situation in Science and Technology and will influence in particular research in MSO. However, basic mathematical research will remain a supporting pillar, despite the shift of emphasis away from pure theoretical research towards mathematical methods in modeling, design and implementation of computational algorithms, adapted to the evolving structures in Information Technology.

2. Strengths and Opportunities

The team specializes in modeling and simulation of processes in geophysics and geo-engineering and has developed a high level of expertise in this field. It is very successful in combining analytical and numerical basic research of high quality with simulation of complex multi-physics problems in complex media. Theory and data based modeling and simulation, as successfully performed by this team, are rather rare also internationally. The team accepted the challenge of modeling and simulation of geological deposition of nuclear waste, a problem of enormous importance, but also very complex due to the complexity of the involved processes and of the geological formations. The team is well prepared for developing models and algorithms adapted to the structure and the potential of the massive parallel Supercomputer recently installed in Ostrava. The Supercomputing Center is responsible in Czech Republic for the supply of science and technology with the resources necessary for High Performance Scientific Computing (HPSC), with not just the hardware but also the software, with the knowhow to develop and implement algorithms on massively parallel systems. This team is urgently needed not only as local node, but also as node in a national network in HPSC. It has the necessary potential and strength.

3. Weaknesses and Threats

A main weakness is the unbalanced age structure. There is a large demand for qualified young scientists at the interface of Mathematics, Computer Science and IT in Supercomputing.

The substantial changes in the Computer technology are requiring a new generation of scientists, not just following the standard tracks of Applied Mathematics and Computer Science. The Institute and the Team are aware of this fact, however the measures so far taken did not yet attract more junior scientists.

HPSC is going to change the future of this team, which just started to reorient itself. The concepts for establishing this direction are so far quite general and need to be specified. The spectrum of the research topics is rather broad up to now, leaving not capacity enough for getting seriously engaged in Mathematics and Computer Science for HPSC.

4. Recommendations

The Commission is aware of the fact, that the team needs also support from the Institute, the

Academy, the Supercomputing Center and outside Institutions to realize in particular the first of the following recommendations:

- increase human resources, in particular to cover the demands arising in high performance computing ,
- improve the conditions attracting highly qualified young scientists (general: challenging scientific program, scientific atmosphere, resources … / personal: appropriate salary, own research group, own resources for starting new projects),
- focus the scientific program and to give a high priority to Computational Sciences and HSCP,
- strengthen the national and international relations in Computational Sciences and HSCP,
- keep balance of basic research in application oriented mathematics and computer science with application dominated research.

5. Detailed evaluations

Declaration on the quality of the results and share in their acquisition
The team is active in the following methodological areas:

1. Robust and efficient numerical methods for solving evolution problems.
2. Numerical methods for porous media flow and poroelasticity.
3. Micromechanics, multi-scale problems.
4. Inverse problems.
5. Parallel algorithms and software.

Specific applications are mainly from geology, geophysics, environmental physics and engineering, material science and engineering.

The Phase I evaluation rated the submitted outputs as follows,
7 % *„world leading“*, 36 % *„internationally excellent“*, 50 % *„recognized internationally“,*
7 % *„recognized nationally“*.

In classifying this positive result, one has to take into account that evaluations are usually harder for interdisciplinary research, in particular if evaluators are more disciplinary oriented. The results presented in the report are mainly from Applied Mathematics and Computational Sciences, whereas the Supercomputing has so far not yet influenced the research to the extend, to be expected in the future. The whole Institute, in particular this Department will undergo important changes. The successful research in MSO in the evaluation period is a good base for research using the potential offered by advanced Information Technology.

Declaration on the involvement of students in research
Several members of the department are successfully contributing to teaching and advising bachelor, master and PhD students. A remarkable number of them finish with a thesis in the research areas of the department. They seem to be well integrated into the activities of the partner universities.

Declaration on societal relevance
The research program is clearly directed to applications. Highly important projects are selected and investigated with the up-to day tools of MSO and using the enormous potential of the Super-

computing Center even more efficiently in the future. Here just some examples are mentioned:
Thermo-mechanical processes in solids; dynamics of damages in materials; hydro-mechanical behavior of bentonite, used for sealing in geo-engineering; storage of waste, in particular nuclear waste.
The department was actively involved in related projects funded through national and European resources.

Declaration on the position in the international and national context
So far the department has been working very successfully, integrated in the Institute for Geonics of CAS, with good scientific national co-operations in particular to teams in Prague, also with growing international links. The national and international visibility and perspectives have substantially increased with the establishment of the Supercomputing Center.

Declaration on the vitality and sustainability
The program of the department requires a strong team, well balanced in age and in expertise. This is not the case at this moment. The age distribution shows the historical dip, observed also in other departments. The Commission discussed measures to be taken with the Director of the Institute, the Board and the representatives of the team.
In order to master the new challenges and to use the large potential, following from the establishment of the Supercomputing Center, the number of scientist, in particular of young scientist, has to be increased. The underrepresentation of young researchers in the group cannot be due to the lack of efforts by the team members to attract students to their research (in which they are quite successful), but must have other structural reasons.

Declaration on the strategy and plans for the future
The research plan is mainly continuing the topics, so far investigated in the department. Not all listed topics have the same importance and offer challenges of the same quality.
Taking into account the personnel resources and the expertise, needed to achieve substantial contributions, a focusing is strongly advised. This holds true for the more method and algorithms oriented topics, but also for the chosen applications. Themes such as
- waste deposits, extraction and use of geothermic energy,
- identification of system parameters from data, often associated with uncertainties,
- analytical and numerical bridging between multiple scales and derivation of effective macroscopic models,
- designing models, numerical algorithms and software, taking into account the structures, the computational power and accessible memory on the different levels of modern computer systems,

require larger groups of scientists with broad expertise. The team should consider focusing on a reduced number of topics to work on or increase its size. It would also be advisable to initiate cooperation in a national network in Computational Sciences and High-Performance-Computing.

Date: December 31, 2015

Commission Chair: Professor Willi Jäger