IT4INNOVATIONS REVIEW 2017

IT4Innovations
national
supercomputing
center

This publication was supported by The Ministry of Education, Youth and Sports from the Large Infrastructures for Research, Experimental Development and Innovations project „IT4Innovations National Supercomputing Center – LM2015070"

IT4INNOVATIONS REVIEW 2017

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MANAGING DIRECTOR'S INTRODUCTION

Dear Readers,

In this review of 2017 we would like to present to you the most important activities and details of the financial management of IT4Innovations National Supercomputing Center for the previous year. I believe that you will find plenty of interesting information that will inform you of the most important events and accomplishments our centre experienced and achieved last year. I also hope that this review will stand as a testament to the value of the overall contribution and importance of our supercomputing centre, as well as of its own in-house research, for the whole of society.

Firstly, I would like to mention that there were significant personnel changes in our centre in 2017. As of the 1st August, I was newly appointed as the Managing Director of IT4Innovations, hence the position of Scientific Director I previously held became vacant. On the 1st September, the newly appointed Rector of VŠB – Technical University of Ostrava, Prof. RNDr. Václav Snášel, Csc., acceded to his office, and therefore left his former position as Head of the Big Data Analysis Laboratory of his own volition. To fill the vacant positions, two open calls were issued, through which Prof. Dr. Ing. Miroslav Vozňák and Prof. Dr. Ing. Tomáš Kozubek were selected as the Head of the Big Data Analysis Laboratory and Scientific Director of IT4Innovations, respectively. As a result of the appointment of the new Scientific Director, the position of Head of the Parallel Algorithms Research Laboratory became vacant. By the end of the year, more open calls for filling the positions of Head of the Parallel Algorithms Research Laboratory, as well as Head of the Infrastructure Research Laboratory, which had already been due, were issued. Within these open calls, Dr. Ing. Tomáš Karásek and Dr. Ing. Lubomír Říha were selected respectively, and on the 1st February 2018 they took up their new roles. I strongly believe that the new IT4Innovations team of key managers will be as successful as the previous ones and will continue to move our centre forward, into the future.

2017 also saw a number of other important events occur which have a significant influence for the further operation and development of our centre. Within the international evaluation of large infrastructures of the Czech Republic, we were awarded the highest possible mark, which means that our

research infrastructure is considered excellent in comparison with other infrastructures worldwide. This evaluation provides a good basis for the justification for the future funding of our infrastructure for the period 2019 to 2022. The approval of the IT4Innovations National Supercomputing Center – Path to Exascale project, funded by Operational Programme Research, Development and Education (OP RDE), in order to modernise and upgrade the Anselm and Salomon supercomputers up to the end of 2021, should be considered the key event of the last year. We were also successful with the Doctoral School for Education in Mathematical Methods and Tools in HPC project, also funded by OP RDE, together with our project partners the Faculty of Mathematics and Physics, Charles University, Prague, and the Institute of Mathematics of the Czech Academy of Sciences, as well as the IT4Innovations Educational and Training Center project. The latter project will lead to building a modern facility for education and training in the immediate vicinity of our centre. We also achieved success with projects within the Horizon 2020 programme. Our following projects were approved for funding; EXPERTISE, CloudiFacturing, and TETRAMAX. Last but not least, we managed to establish collaborations with several new industrial partners.

Under the name of our centre, the regular international High Performance Computing in Science and Engineering conference was organized, taking place at Soláň as in previous years. Within the pan-European research infrastructure Partnership for Advanced Computing in Europe (PRACE), we received the status of the PRACE Training Centre and organized an introductory training week within the Summer of HPC programme. For the first time, our centre served as the venue for organizing the IT4Innovations Users Conference held along with the annual Scientific Conference of the IT4Innovations Centre of Excellence. At this conference, the IT4Innovations Users Council was also established. Moreover, we organized a wide range of workshops and excursions attended by more than 1700 visitors of all ages. I am very pleased that there is still strong interest in our centre, mainly from young people, who leave our centre enriched with the knowledge that supercomputers are not futuristic science fiction, but current science fact, and a real tool in our present, used for excellent research and industrial innovations.

A similarly pleasing fact is that users' interest in our computing infrastructure continues to increase. The capacity of our systems is currently fully utilized, and we are not able to meet all demand from our user base. The currently proceeding tender for the Anselm cluster upgrade will hopefully, albeit at least partially, solve this situation.

I humbly believe that we can justly be proud of all the above-mentioned successful projects, and my thanks go to all those who participated in them to a greater or lesser degree. However, I would also like to express my thanks to those, whose results were not so fortunate as to be included in this introduction, or who participated only indirectly by means of, e.g., technical or administrative support. Their work effort and engagement also deserve our appreciation despite their names not being included in those achievements. It is highly important for us to establish and continuously develop a strong team, as only in this way will we be able to maintain the prestigious position of our centre at home and abroad.

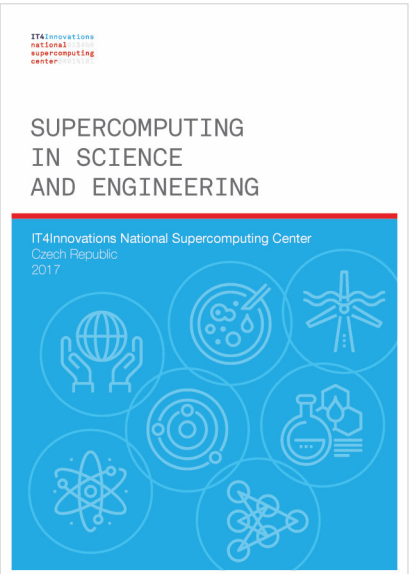
Vít Vondrák
Managing Director of IT4Innovations

IMPORTANT EVENTS IN 2017

IT4Innovations is currently the only national large research infrastructure in the field of High Performance Computing (HPC) in the Czech Republic, and it is our ambition to continue to play this leading role into the future. In 2017, the **IT4Innovations National Supercomputing Centre – Path to Exascale** project, the objective of which is to modernize the existing supercomputers and extend our own research in new directions, was approved for funding from the Operational Programme Research, Development and Education (OP RDE). In addition, the following two projects were also approved from OP RDE. The **Doctoral School for Education in Mathematical Methods and Tools in HPC** project will allow students of doctoral study programmes included in the Doctoral School to share a mutual supply of subjects and participate in joint activities. Partners of the project are the Charles University in Prague and the Czech Academy of Sciences. Concurrently double-degree doctoral study programmes with the Swiss Università della Svizzera italiana and the French Université de Toulouse III Paul Sabatier will be established.

The third project, also funded by OP RDE, will support the building of the **IT4Innovations Educational Training Center**. The new building, furnished with an auditorium and three lecture rooms, will provide a base for research-oriented study programmes focused on computational sciences.

Last year we also achieved success in the area of international research projects. Within Horizon 2020 - the Framework Programme for Research and Innovation in the European Union, three new international projects we participate in were approved. We have become members of the prestigious consortium of the international **EXPERTISE** (Experiments and High Performance Computing for Turbine Mechanical Integrity and Structural Dynamics in Europe) project, which provides a platform for collaboration between the new generation of mechanical engineers and researchers, for the research and development of turbines. The objective of the **TETRAMAX** (Technology Transfer via Multinational Application Experiments) project is to facilitate provision of new innovative technologies to European industry by establishing a specialized network of competence centres. Within the **CloudiFacturing** (Cloudification of Production Engineering for Predictive Digital Manufacturing) project, optimization of manufacturing processes and productivity using modelling and simulations by means of HPC/cloud technologies is offered.



Publication Supercomputing in Science and Engineering

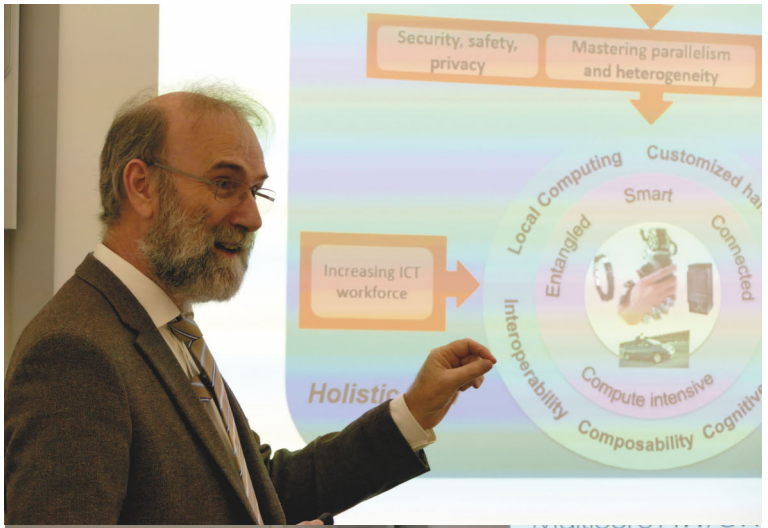
In 2017, we published the book **Supercomputing in Science and Engineering** (ISBN 978-80-248-4037-6). It is the first collection of extended abstracts of 62 selected research projects, which used the IT4Innovations infrastructure. In this publication, projects in fields such as astrophysics, computational sciences, Earth sciences, engineering, chemistry and material engineering, and biosciences and physics can be found. As well as IT4Innovations authors, other important educational and research institutions contributed 40 extended abstracts altogether to this publication, namely, for example, the Czech Academy of Sciences, the Czech Technical Unviersity in Prague, Charles University, the Brno University of Technology and Masaryk University.

In May 2017, we organized the third **High Performance Computing in Science and Engineering** (HPCSE) conference. The latest research results in the fields of applied mathematics, numerical linear algebra, optimization methods, computational sciences and HPC were presented there. Almost 100 experts and students from the Czech Republic and other countries participated in the HPCSE conference this time.

HPCSE Conference, May 2017

In November 2017, the 1st IT4Innovations Users Conference, attended by 121 participants, was held at IT4Innovations. The invited speakers included researchers from the Czech Academy of Sciences, Charles University in Prague, and the Czech Technical University in Prague (CTU), all of whom use the IT4Innovations infrastructure. **Dr. Paolo Nicolini** from the Faculty of Electrical Engineering of CTU in Prague was elected the Chairman of the Executive Board for the IT4I Users Council.

1st Users Conference of IT4Innovations, Novemeber 2017



In February 2017 our centre proudly hosted the first workshop of the international HiPEAC network to take place in the Czech Republic. The HiPEAC network gathers experts in HPC and embedded systems. Within the first workshop in the Czech Republic, we were visited by the representatives of the HiPEAC network, Koen De Bosschere and Rainer Leupers.

HiPEAC workshop at IT4Innovations, February 2017

In 2017, nine training activities were organised, and were attended by a total of 227 participants. We were awarded the status of the PRACE Training Centre. Seven countries, or partners representing these countries in PRACE, were applying for this status as well. To our delight, the PRACE Panel of Experts chose IT4Innovations, which ranked highest in the evaluation.

Events aimed at the general public which were held at our centre this year attracted almost 1700 visitors. These events included, for example, excursions for pupils, students, companies, and popularisation events such as the Researchers' Night.

Excursions and educational events for the public

IT4INNOVATIONS PROFILE

IT4Innovations National Supercomputing Center at VŠB – Technical University of Ostrava represents a strategic large research infrastructure in the Czech Republic. The National Supercomputing Center provides state-of-the-art supercomputing technology and services, and conducts excellent research in the fields of high performance computing (HPC) and data analysis (HPDA). Since 2011, IT4Innovations has been a member of Partnership for Advanced Computing in Europe (PRACE), the prestigious pan-European research infrastructure, the objective of which is to increase the competitiveness of European science, research, and industry. In 2016, we became a member of the European Technological Platform for HPC (ETP4HPC), which is focused on defining research priorities in the field of supercomputing.

Our main research areas include big data processing and analysis, development of parallel scalable algorithms and libraries, supercomputing technology development, solving computationally demanding real engineering problems, and modelling for nanotechnologies. For the Czech scientific community, we provide an access to powerful computing resources, and a wide range of training sessions aimed at acquiring the knowledge needed to efficiently use our supercomputing infrastructure. We also care for the future by educating the next generation of experts in utilizing supercomputers for solving computationally demanding problems in basic research as well as in applied sciences.

Mission

Our mission is to deliver scientifically excellent and industry-relevant research in the fields of high performance computing. We provide state-of-the-art technology and expertise in high performance computing, and make it available for Czech as well as international research teams from academia and industry.

Vision

Our vision is to become the top European Centre of Excellence in IT with the emphasis on high performance computing. With our research, know-how, and infrastructure, we aspire to improve the quality of life, increase the competitiveness of the industrial sector, and promote interdisciplinary collaboration across the fields of high-performance computing, and other scientific and technical disciplines.

Research Infrastructure Advisory Board of IT4Innovations National Supercomputing Center / Scientific Council of IT4Innovations Centre of Excellence

Members:
- Doc. Dr. Mgr. Vít Vondrák
- Prof. Dr. Michael Cada
- Prof. Jean-Christophe Desplat
- Prof. Dr. Ing. Petr Berka
- Prof. Dr. Peter Arbenz
- Doc. Dr. Ing. Petr Cintula
- Prof. Dr. Dipl.-Ing. Ulrich Bodenhofer
- Prof. Dr. Kenneth Ruud
- Prof. Dr. Arndt Bode
- Prof. Dr. hab. inz. Roman Wyrzykowski

Scientific Council of IT4Innovations, University Institute of VŠB – Technical University of Ostrava

Chairman: Doc. Dr. Mgr. Vít Vondrák

Members:
- Dr. Mgr. Branislav Jansík
- Dr. Ing. Jan Martinovič
- Prof. Dr. Ing. Tomáš Kozubek
- Prof. Dr. Ing. Jaromír Pištora
- Doc. Dr. Ing. Pavel Krömer
- Prof. Dr. Ing. Jan Holub
- Prof. Dr. Ing. Pavel Tvrdík
- Doc. Dr. RNDr. Stanislav Hledík
- Prof. Dr. RNDr. Jaroslav Pokorný
- Doc. Dr. RNDr. Arnošt Komárek
- Prof. Dr. Ing. Viera Stopjaková
- Dr. Ing. Martin Palkovič

In 2017, we also continued in collaboration with the partners of the IT4Innovations Centre of Excellence project – the University of Ostrava, the Silesian University in Opava, Brno University of Technology, and the Institute of Geonics of the Czech Academy of Sciences. Since 2016, we have been jointly implementing the IT4Innovations Excellence in Science project, which is funded by the National Programme of Sustainability II (NPS II). Supervision of this project as well as the sustainability of the original Centre of Excellence project is ensured by the Managing Board.

Supervisory Board

Chairman: Ing. Evžen Tošenovský, Dr.h.c.

Vice-chairman: Doc. Dr. Mgr. Pavel Drozd

Members:
- Prof. Dr. Ing. Ivo Vondrák
- Prof. Dr. Ing. Petr Noskievič
- Ing. Miroslav Murin, FCCA
- Prof. Dr. Ing. Pavel Zemčík
- Ing. Leoš Dvořák
- Doc. Dr. Ing. Pavel Tuleja
- Prof. Dr. Ing. Miroslav Tůma

ADMINISTRATIVE AND FINANCIAL REVIEW

Management of IT4Innovations as of 1st November 2017

Managing Director of IT4Innovations
Vít Vondrák

Administration
Radim Mrázek

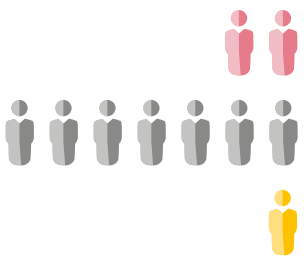
Research and Development
Tomáš Kozubek

Supercomputing services
Branislav Jansík

Until 31st July 2017, the function of the Managing Director of IT4Innovations National Supercomputing Center was held by Dr. Ing. Martin Palkovič. The current Managing Director of IT4Innovations is Doc. Dr. Mgr. Vít Vondrák (the former Scientific Director of IT4Innovations), who was appointed to the function on 1st August 2017. Since 1st November 2017, the function of the Scientific Director has been held by Prof. Dr. Ing. Tomáš Kozubek.

Employees of IT4Innovations

Employees of IT4Innovations by divisions in full time equivalent (FTE), 132.7 FTE in total



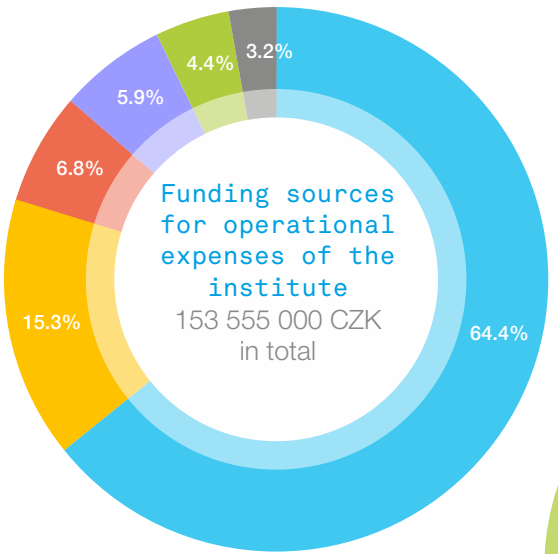
21 % Management and Administration

68 % Research and Development

11 % Supercomputing services

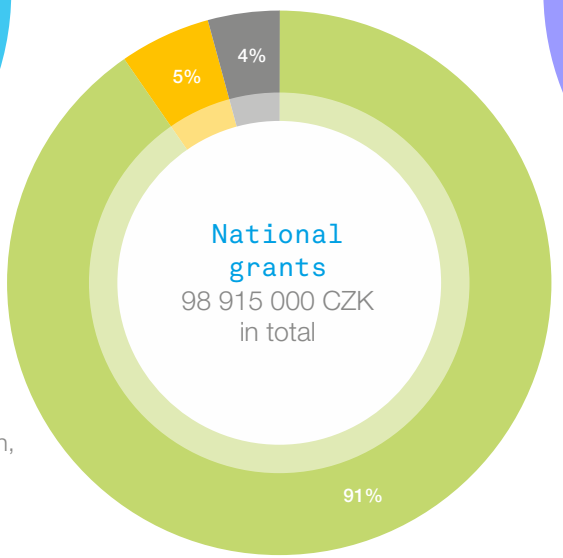
Sources of funding

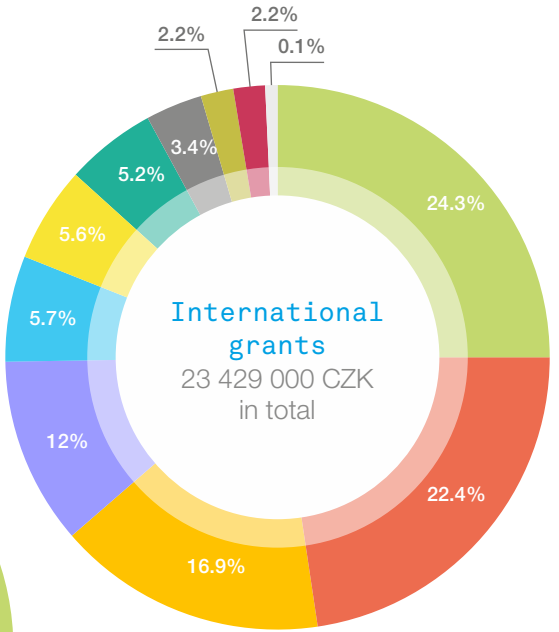
In 2017, the overall budget of the institute was CZK 153,555,000. The largest share of the funding sources for operational expenses of the institute was contributed by national grants (targeted support, 64.4 %). Other funding sources for operational expenses of the institute included international grants (15.3 %), institutional support (6.8 %), Operational Programme Research, Development and Education (4.4 %), and contract research together with renting out computational resources (3.2 %) as well as our own sources (5.9 %), donations, and income from contractual fines.



- National grants
- International grants
- Institutional support
- Others
- Operational Programme Research, Development, and Education
- Contract research and renting computational resources

- Ministry of Education, Youth and Sports of the Czech Republic (13 projects)
- Technology Agency of the Czech Republic (3 projects)
- Grant Agency of the Czech Republic (3 projects)

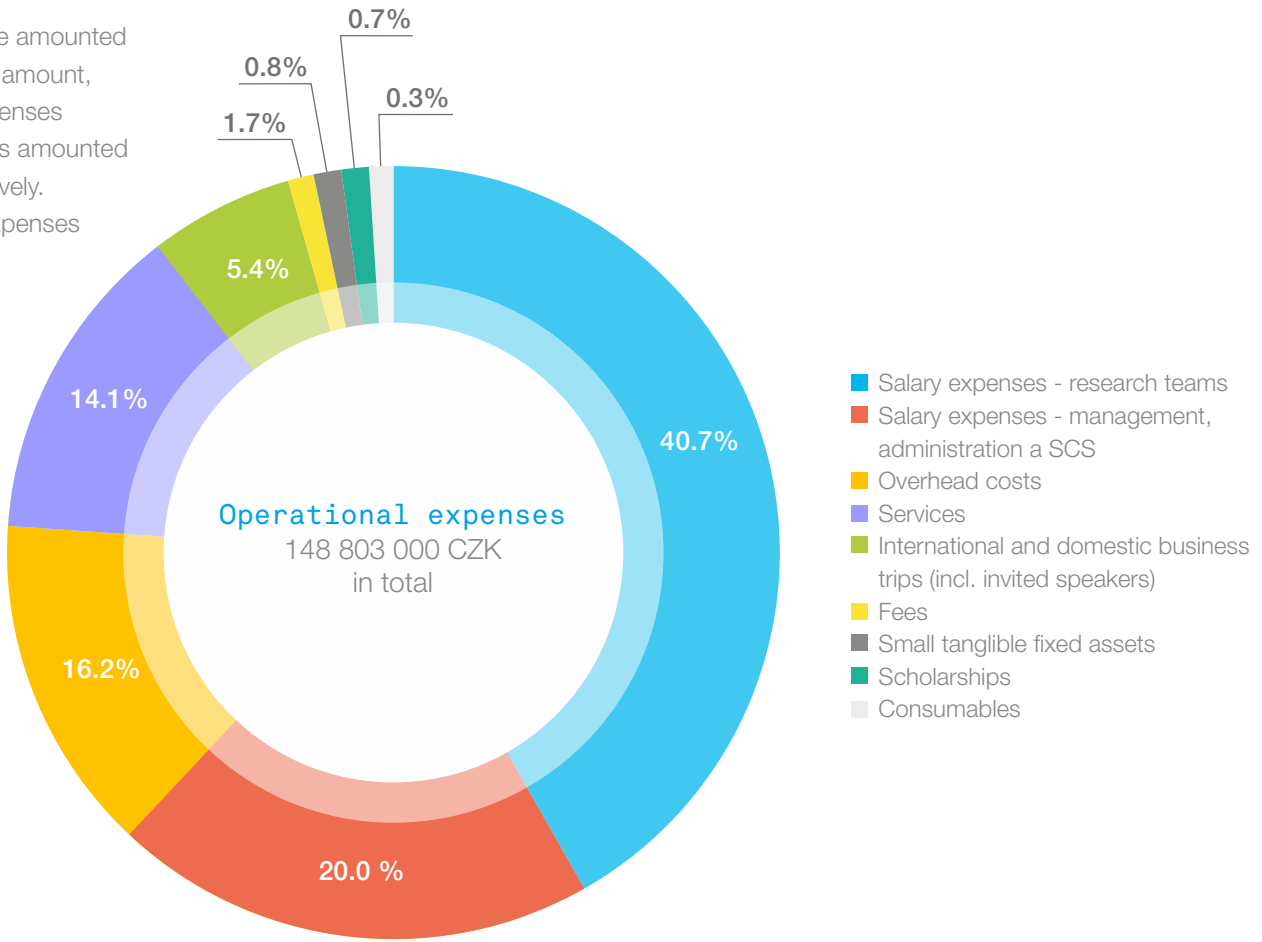




- READEX
- ExCAPE
- ANTAREX
- PRACE, 5th implementation phase
- LOWBRASYS
- PRACE, 4th implementation phase
- InnoHPC
- SESAME – NET
- CloudiFacturing
- TETRAMAX
- EXPERTISE

Operational and capital expenditures

The total expenses of the institute amounted to CZK 149,022,000. Within this amount, non-investment (operational) expenses and investment (capital) expenses amounted to 99.85 % and 0.15 %, respectively. The largest part of operational expenses included personnel expenses, overhead expenses, and services (91 %).



Summary of all grants

NATIONAL GRANTS

Projects supported by the Ministry of Education, Youth and Sports of the Czech Republic

Large Infrastructures project

- IT4Innovations National Supercomputing Center

National Programme of Sustainability II

- IT4Innovations Excellence in Science

Grants for specific university research

- Creation of rendering service
- Terahertz spectroscopy of photonic structures using advanced materials
- Massively parallel modelling of strongly nonlinear processes in mechanics
- Efficient implementation of the boundary element method III
- Numerical methods for modelling environmental processes
- Modelling of collision processes in low-temperature plasma
- PERMON toolbox development III
- Optimization of machine-learning algorithms for an HPC platform
- Solution of graph problems on uncertainty time-space graphs using HPC
- Thermal expansion of Fe-Ti alloys

Project supported by the Programme for funding projects of multilateral scientific and technical cooperation in the Danube region

- Complex study of effects in low-dimensional quantum spin systems

Projects supported by the Grant Agency of the Czech Republic

- New nonlinear and magneto-optical phenomena in periodic structures
- Efficient lifetime estimation techniques for general multiaxial loading
- Novel fuel materials for Generation IV nuclear reactors

Projects supported by the Technology Agency of the Czech Republic

- Centre of Competence for molecular diagnostics and personalized medicine
- Parallelized reaction-transport model of contamination spread in groundwater
- Transport Systems Development Centre

Projects of Operational Programme Research, Development, and Education

- IT4Innovations National Supercomputing Center – path to exascale
- Doctoral School for Education in Mathematical Methods and Tools in HPC
- IT4Innovations Educational Training Center
- Technique for the Future

INTERNATIONAL GRANTS

Projects of the 8th Framework Programme for Research and Innovations of the European Union – Horizon 2020

- PRACE-4IP – Partnership for Advanced Computing in Europe, 4th implementation phase
- SESAME Net – Supercomputing Expertise for Small and Medium Enterprise Network
- ExCAPE – Exascale Compound Activity Prediction Engine
- ANTAREX – AutoTuning and Adaptivity appRoach for Energy efficient eXascale HPC systems
- READEX – Runtime Exploitation of Application Dynamism for Energy-efficient eXascale computing
- LOWBRASYS – A Low Environment Impact Brake System
- EXPERTISE – Experiments and High Performance Computing for Turbine Mechanical Integrity and Structural Dynamics in Europe
- TETRAMAX – Technology Transfer via Multinational Application Experiments
- CloudiFacturing – Cloudification of Production Engineering for Predictive Digital Manufacturing
- PRACE-5IP – Partnership for Advanced Computing in Europe, 5th implementation phase

Project of the Interreg Danube Transnational Programme (EU funds)

- InnoHPC – High-Performance Computing for Effective Innovation in the Danube Region

Project of the European Space Agency

- Urban TEP – Urban Thematic Exploitation Platform

Other projects

- CzeBaCCA – Czech-Bavarian Competence Team for Supercomputing Applications
- IPCC - Intel® Parallel Computing Center at IT4Innovations National Supercomputing Center

The International Energy Club visited IT4Innovations in September 2017


SUPERCOMPUTING SERVICES

SUPERCOMPUTING SERVICES

IT4Innovations National Supercomputing Center provides Czech and foreign research teams from both academia and industry with state-of-the-art HPC technologies and services. IT4Innovations is currently operating two supercomputers – Anselm and Salomon.

Technical specifications of the supercomputers

	ANSELM	SALOMON
Put into operation	Spring 2013	Summer 2015, 87th on the TOP500 list of the most powerful supercomputers in the world (November 2017)
Peak performance	94 Tflop/s	2011 Tflop/s
Operating system	RedHat Linux 64bit 6.x	RedHat Linux 64bit 6.x, CentOS 64bit 6.x
Nodes	209	1008
CPU	2x Intel SandyBridge 8 cores, 2.3 / 2.4 GHz, 3344 cores in total	2x Intel Haswell 12 cores, 2.5 GHz, 24192 cores in total
RAM per computing nodes	64 GB / 96 GB / 512 GB	128 GB / 3.25 TB (UV node)
GPU accelerators	23x NVIDIA Tesla Kepler K20	N/A
MIC accelerators	4x Intel Xeon Phi 5110P	864x Intel Xeon Phi 7120P, 61 cores each, 52704 cores in total
Storage	320 TiB home (2 GB/s), 146 TiB scratch (6 GB/s)	500 TiB home (6 GB/s), 1638 TiB scratch (30 GB/s)
Interconnection	Infiniband QDR 40 Gb/s	Infiniband FDR 56 Gb/s

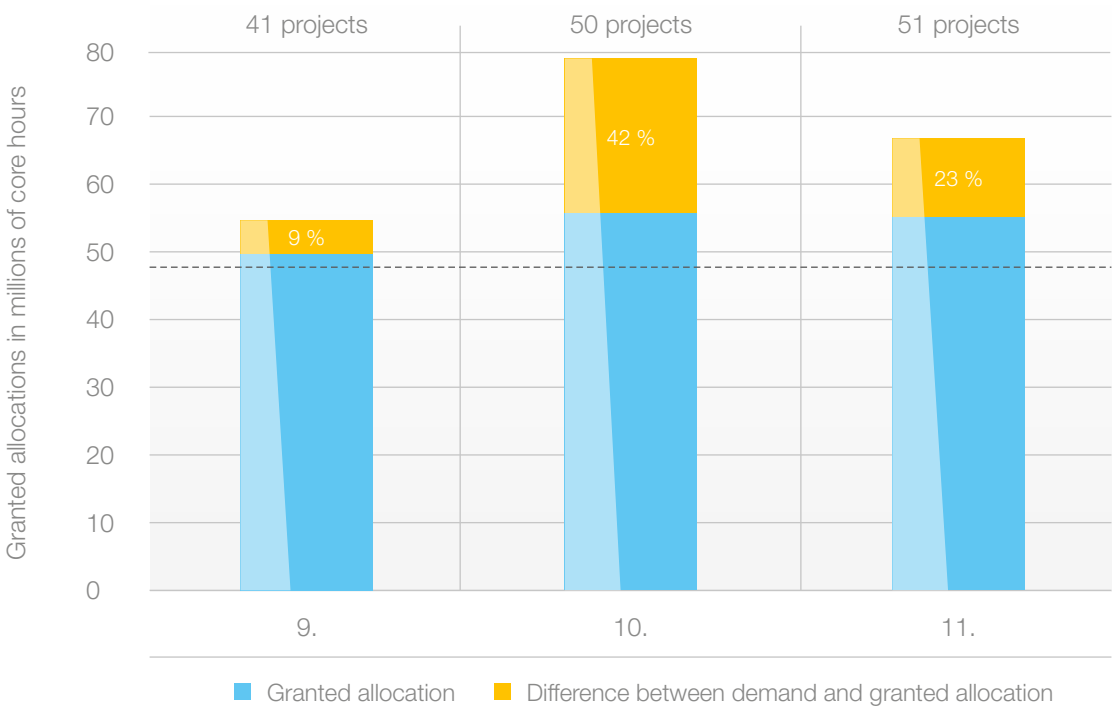
In 2017, the IT4Innovations National Supercomputing Centre – Path to Exascale project, the objective of which is to modernize the existing supercomputers and extend its own research activities in new directions, was approved for funding from the Operational Programme Research, Development and Education (OP RDE). The project has been being implemented since September 2017. Almost 80 % of the total expenses of the project are dedicated to modernization of the existing supercomputers and the related infrastructure. The remaining funding resources will be used to support new research directions at IT4Innovations. By the end of 2018, users of IT4Innovations computational resources will benefit from the upgraded Anselm supercomputer, and in 2020, also the upgraded Salomon supercomputer.

Computational resources allocation

The computational resources of IT4Innovations are dedicated for solving problems in research and development conducted by academic and research institutions. Unused capacity can be freed up for the development of collaboration between academia and industry, and for the purpose of independent use by industrial enterprises.

Institutions can apply for computational resources within Open Access Grant Competitions. These are announced three times a year. In 2017, 160,350,384 core hours were allocated within three Open Access Grant Competitions, and distributed among 142 research projects enhancing Czech science.

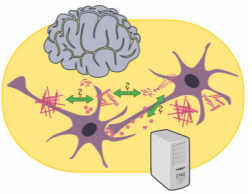
Open Access Grant Competitions in 2017



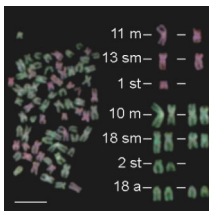
The computational resources earmarked for an Open Access Grant Competition amount to 48 million core hours. In 2016 and 2017, the excess demand for core hours over the available capacity amounted to almost 21 % and more than 39 %, respectively. This difference is compensated by the reserves available through the Director's Discretion scheme as well as the Anselm system computational resources. The Allocation Committee found most of the submitted applications scientifically and technically thoroughly elaborated. However, for the reason of insufficient capacity, the computational resources awarded to each project had to be reduced.

Results of the 9th Open Acces Grant Competition in Newsletter Q1/2017

Orbital floor fracture and the project of Dr. Ing. Petr Strakoš

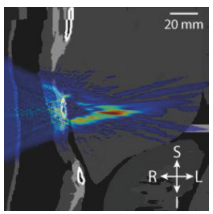


Neurons and the project of Dr. RNDr. Mgr. Jozef Hritz

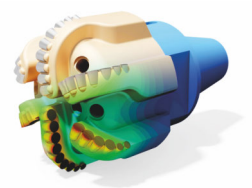


Chromosomes of the hybrid of Cobitis taenia and Cobitis elongatoides and the project of Dr. Mgr. Karel Janko

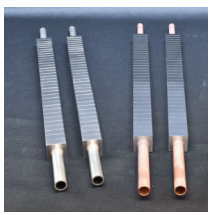
Results of the 10th Open Acces Grant Competition in Newsletter Q2/2017



Sonication in the liver with strong rib distortion and the project of Doc. Dr. Ing. Jiří Jaroš

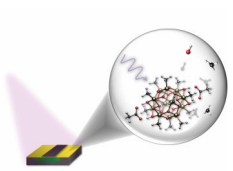


Drill bit and the project of Dr. Ing. Tomáš Brzobohatý

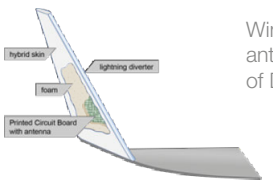


Prototypes of the actively cooled diverter components for the ITER Tokamak that will be tested in the WEST Tokamak and the project of Dr. Mgr. Michael Komm

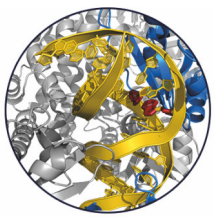
Results of the 11th Open Access Grant Competition in Newsletter Q4/2017



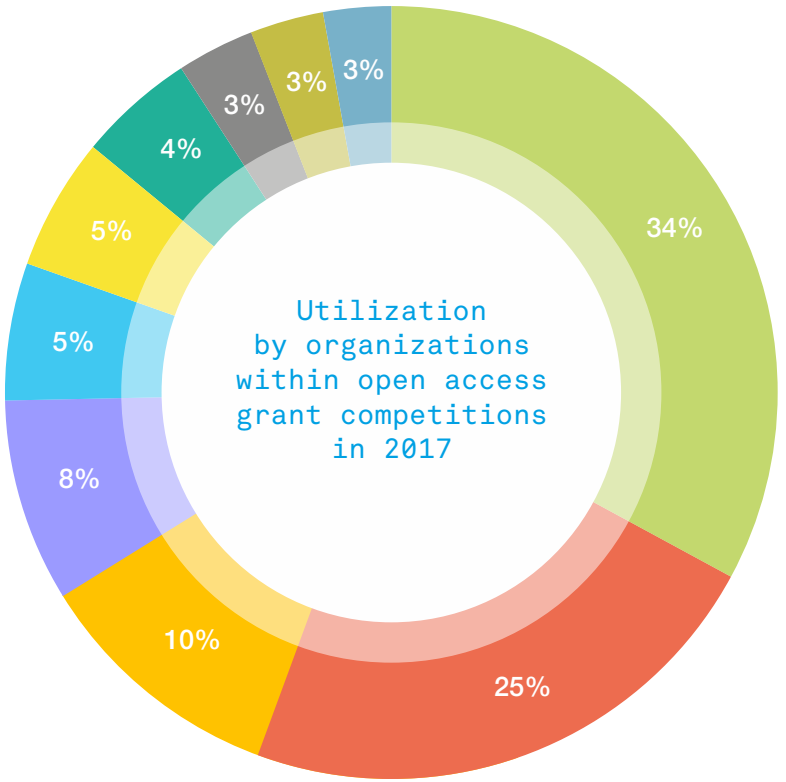
How can targeted high-energy radiation change material and the project of Prof. Dr. RNDr. Petr Slavíček



Winglet with an integrated antenna and the project of Dr. Ing. Petr Vrchota



Repair of damaged base pairing in DNA and the project of Dr. RNDr. Petr Kulhánek

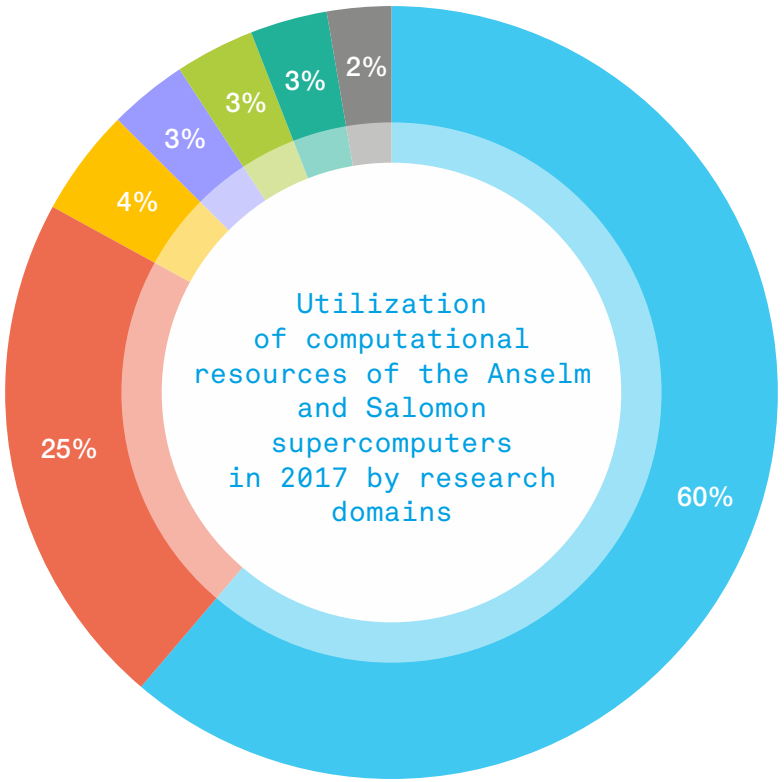


Within the Open Access Grant Competitions of 2017, a total of 37 projects of applicants from VŠB – Technical University of Ostrava and thus IT4Innovations, were awarded computational resources. Seven projects were led by researchers from the Faculty of Electrical Engineering and Computer Science, the Faculty of Mechanical Engineering, the Faculty of Civil Engineering, and the Faculty of Metallurgy and Materials Engineering.

Concerning the external research institutions using the IT4Innovations infrastructure, most of the computational resources were allocated to the projects of researchers affiliated with the Czech Academy of Sciences (CAS). In 2017, they were allocated computational resources for 28 projects in total. More than 21 million core hours were allocated to 8 projects from the Institute of Organic Chemistry and Biochemistry. Almost 10 million core hours were allocated to seven projects of researchers from J. Heyrovsky Institute of Physical Chemistry.

The third institution making most use of the IT4Innovations infrastructure in 2017 is Charles University in Prague with its researchers being allocated more than 16 million core hours.

- VŠB – Technical University of Ostrava (37 projects)
- The Czech Academy of Sciences (28 projects)
- Charles University (27 projects)
- CEITEC (9 projects)
- Brno University of Technology (9 projects)
- Czech Technical University in Prague (8 projects)
- University of Ostrava (4 projects)
- Masaryk University (2 projects)
- University of Chemistry and Technology in Prague (5 projects)
- Others (13 projects)



- Material sciences (42 projects)
- Biosciences (31 projects)
- Engineering (21 projects)
- Computational sciences (14 projects)
- Applied mathematics (11 projects)
- Physics and astronomy (9 projects)
- Earth sciences (14 projects)

The lists of projects which were awarded computational resources within the Open Access Grant Competitions in 2017 in order 9th, 10th, 11th.

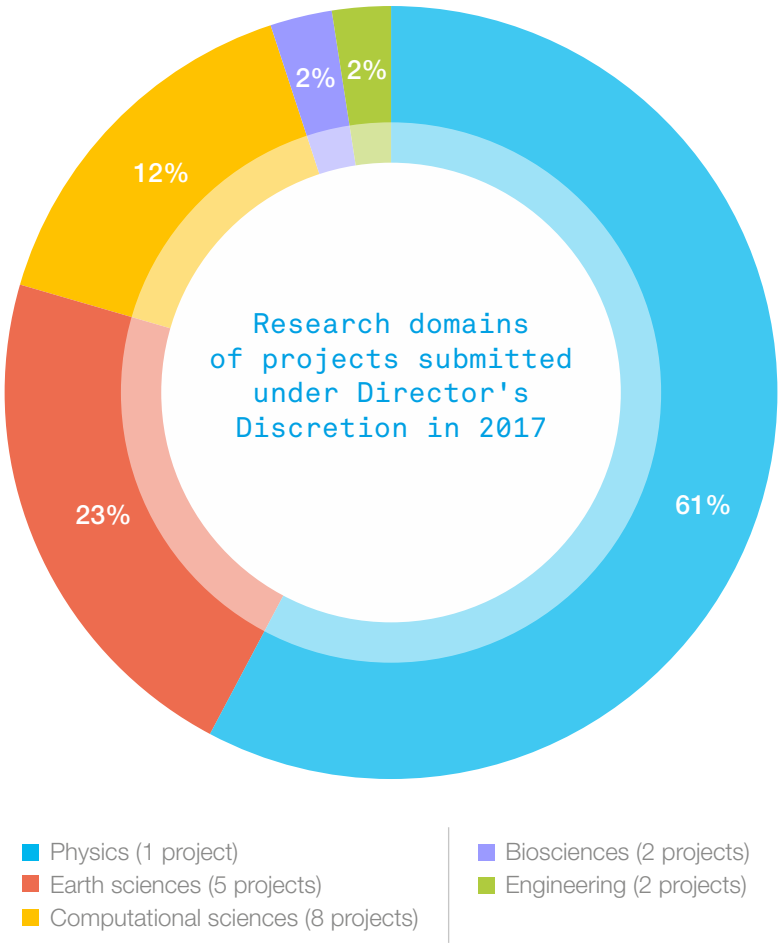
Computational resources can also be granted upon request through the Director's Discretion scheme. An application can be submitted at any time. The computational resources are allocated irregularly based on an evaluation by the IT4Innovations management. Representatives from both commercial and non-commercial sectors can apply in case Open Access Grant Competitions cannot be used. Within the Director's Discretion scheme in 2017, a total of 18 projects were allocated 1,951,600 core hours.

Users of computational resources

The number of active users was 723 in total in 2017.

Our technical support received 1600 queries and requests in 2017, 1598 of which were successfully resolved. Two requests were rejected.

Internal response time (24 h for first response) was observed in 99.87 % of queries. Internal closure time, which should not be longer than 30 days, was observed in 99.75 % of queries.



Projects

Several national and international grants help us secure the development of our supercomputing infrastructure. The most important one is the grant from the Ministry of Education, Youth and Sports of the Czech Republic – IT4Innovations National Supercomputing Center, which is funded from sources dedicated to supporting large infrastructures for research, experimental development, and innovation. Important international projects we are involved in, thanks to our Partnership for Advanced Computing in Europe (PRACE) membership, are PRACE infrastructure projects. In the year 2017, the fifth project called PRACE-5IP was realized.

NATIONAL GRANTS

IT4Innovations National Supercomputing Center (2016–2019)

Project ID: LM2015070
(Large Infrastructures for Research and Development for Innovations project)
Principal Investigator: Dr. Ing. Martin Palkovič
(from the 1st January 2018: Doc. Dr. Mgr. Vít Vondrák)

The objective of the project is to operate the most powerful, state-of-the-art supercomputing systems in the Czech Republic and provide open access to these resources based on research excellence.

IT4Innovations is currently operating the most powerful computing system in the Czech Republic, with a theoretical peak performance of 2 PFLOPS, and a smaller system with theoretical peak performance of 94 TFLOPS.

Necessary for providing the aforementioned computing capacities is the operation of the related infrastructure (power supply, cooling, safety, fire protection, etc.), as well as the user support and the management of computing and infrastructure systems. The supercomputer infrastructure also includes research activities that streamline its operation and extend its use to the user. The educational and training activities that are open to the broad scientific community of the Czech Republic also contribute to effective use of the infrastructure.
http://www.msmt.cz/vyzkum-a-vyvoj-2/cestovni-mapa-cr-velkych-infrastruktur-pro-vyzkum

OPERATIONAL PROGRAMME RESEARCH, DEVELOPMENT AND EDUCATION

IT4Innovations National Supercomputing Center – path to exascale (2017–2021)

Project ID: EF16_013/0001791
(call no. 02_16_013 Research infrastructures)
Principal Investigator: Dr. Mgr. Branislav Jansík

The objective of this project is to upgrade and modernize the research infrastructure of IT4Innovations so as to minimally maintain the existing technological level of HPC in the Czech Republic in comparison with developed, particularly European, countries. The activities of this project are aimed at modernizing the current Anselm supercomputer in 2018, and supercomputer Salomon in 2020.

Additional objectives of the project are also the support of high-quality research across the wider academic community in the Czech Republic, and the expansion of existing research activities in IT4Innovations in the field of modelling photonic and spin-photonic structures, design of progressive materials based on electronic structure calculations, and analysis of bioimages using HPC. For the IT4Innovations infrastructure, our own in-house research is an important source of HPC expertise, which is reflected in services provided by this infrastructure to its users.

INTERNATIONAL GRANTS

PRACE-4IP – Partnership for Advanced Computing in Europe, 4th implementation phase (2015–2017)
Project ID: 653838
(H2020-EINFRA-2014-2 Call)
Principal Investigator: Doc. Dr. Mgr. Vít Vondrák
http://www.prace-ri.eu/prace-4ip/

PRACE-5IP – Partnership for Advanced Computing in Europe, 5th implementation phase (2017–2019)
Project ID: 730913
(H2020-EINFRA-2016-1 Call)
Principal Investigator: Doc. Dr. Mgr. Vít Vondrák
http://www.prace-ri.eu/prace-5ip/

The objective of the PRACE projects is to build on successful implementation of the previous PRACE projects, whose task was to implement the European HPC infrastructure and to continue to develop supercomputing cooperation to strengthen the competitiveness of European science, research and industry.

CzeBaCCA – Czech-Bavarian Competence Team for Supercomputing Applications

CzeBaCCA, initiated on 1st January 2016, having the goal of creating a Czech-Bavarian competence team for supercomputing applications, and funded mainly by the German Federal Ministry of Education and Research, responded to the ever-increasing complexity of modern supercomputers and related necessity of efficient support of experts in various areas of application. It was based on the excellent collaboration of IT4Innovations National Supercomputing Center with the Leibniz Supercomputing Center (LRZ) and the Technical University of Munich.

In 2017, the following workshops were successfully organized within the CzeBaCCA project in order to facilitate sharing of experience and knowledge in the given area:

In Ostrava:
- PRACE PATC Course: Intel MIC Programming Workshop
- Scientific Workshop: High performance computing in atmosphere modelling and air related environmental hazards

In Garching:
- PRACE PATC Course: Intel MIC Programming Workshop
- Scientific Workshop: HPC for natural hazard assessment and disaster mitigation

Although the CzeBaCCA project finished in July 2017, the collaboration, in the sense of the last objective mentioned above, continues in various forms. In the area of education, for example, IT4Innovations, together with its German partners, plans to organize a week-long VI-HPS Tuning Workshop in April in 2018, which will be an important event dedicated to practical optimization of user codes.
https://www.lrz.de/forschung/projekte/forschung-hpc/CzeBaCCA/

SESAME - NET – Supercomputing Expertise for Small and Medium Enterprise Network (2015–2017)
Project ID: 654416 (H2020-EINFRA-2014-2 Call)
Principal Investigator: Dr. Ing. Tomáš Karásek

The objective of this project was to establish a network of centres mutually cooperating with, and supporting small and medium-sized industrial enterprises in exploitation of HPC for their development. Within the scope of this project, various educational materials were prepared, which are now available to all interested parties.
https://sesamenet.eu

InnoHPC – High Performance Computing for Effective Innovation in the Danube Region (2017–2019)
Project ID: DTP1-1-260-1.1
(INTERREG/Danube region programme, 1st Call)
Principal Investigator: Dr. Ing. Tomáš Karásek

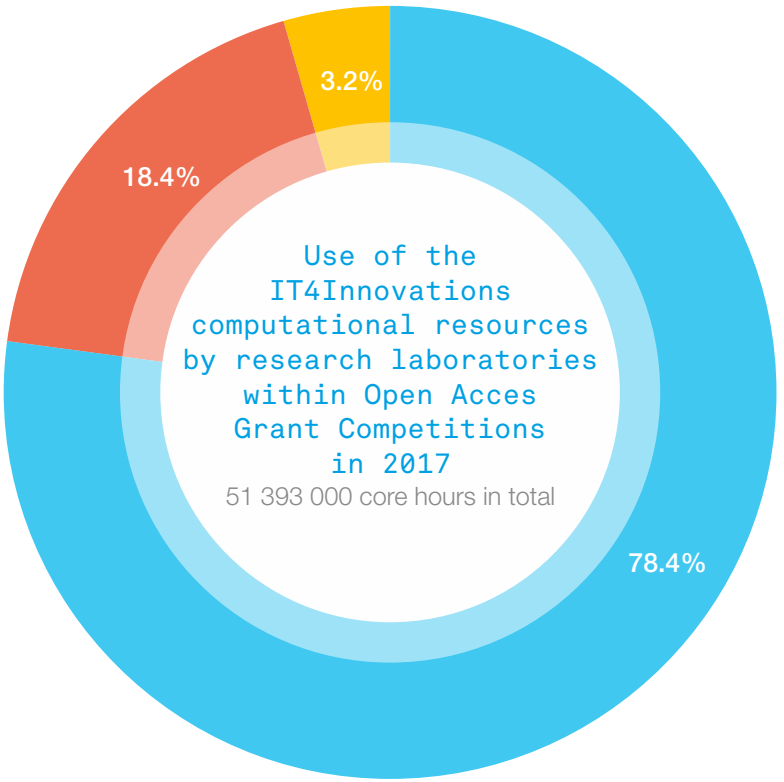
The objective of the InnoHPC project is to design a transnational HPC platform for developing cooperation of research institutions with small and medium-sized enterprises. The participating enterprises will be allowed access to supercomputing infrastructures. The participating research institutions, on the other hand, will gain an opportunity to collaborate in solving real world problems and use their entrepreneurial potential.
http://www.interreg-danube.eu/approved-projects/innohpc

RESEARCH AND DEVELOPMENT

RESEARCH AND DEVELOPMENT

The key IT4Innovations research topics include advanced data processing and analysis, parallel scalable algorithms development, solving challenging engineering problems, and modelling for nanotechnologies and infrastructure research. The research in these areas is concentrated into 5 laboratories. The **Parallel Algorithms Research Laboratory** is focused on developing its own in-house scalable algorithms and sofware libraries, which are used for collaboration with both academic and industrial partners. The **Advanced Data Analysis and Simulations Laboratory** is focused on big data processing and analysis, that are part of advanced data-based computer simulations. The **Modelling for Nanotechnologies Laboratory** is focused on designing novel materials using electronic structure calculations. The **Big Data Analysis Laboratory** is focused on uncovering information hidden in large data sets. In January 2017, we also newly established the Infrastructure Research Laboratory. This laboratory has enhanced our own in-house infrastructure research and is focused on developing methods for innovative use, operation, and monitoring of the computing infrastructure.

Laboratory	Acronym	Head of Laboratory	FTE
Parallel Algorithms Research Laboratory	PAR	Prof. Tomáš Kozubek (from 1st February 2018: Dr. Tomáš Karásek)	37.58
Advanced Data Analysis and Simulations Laboratory	ADAS	Dr. Jan Martinovič	31.10
Modelling for Nanotechnologies Laboratory	NANO	Prof. Jaromír Pištora	9.60
Big Data Analysis Laboratory	BIGDATA	Prof. Miroslav Vozňák	5.11
Infrastructure Research Laboratory	INFRA	Dr. Branislav Jansík (from 1st February 2018: Dr. Lubomír Říha)	7.26



In 2017, IT4Innovations research projects were allocated to a total amount of 51,393,000 core hours in open access grant competitions, which is 32 % of the total allocation.

- Modelling for Nanotechnologies Laboratory
- Parallel Algorithms Research Laboratory
- Advanced Data Analysis and Simulations Laboratory

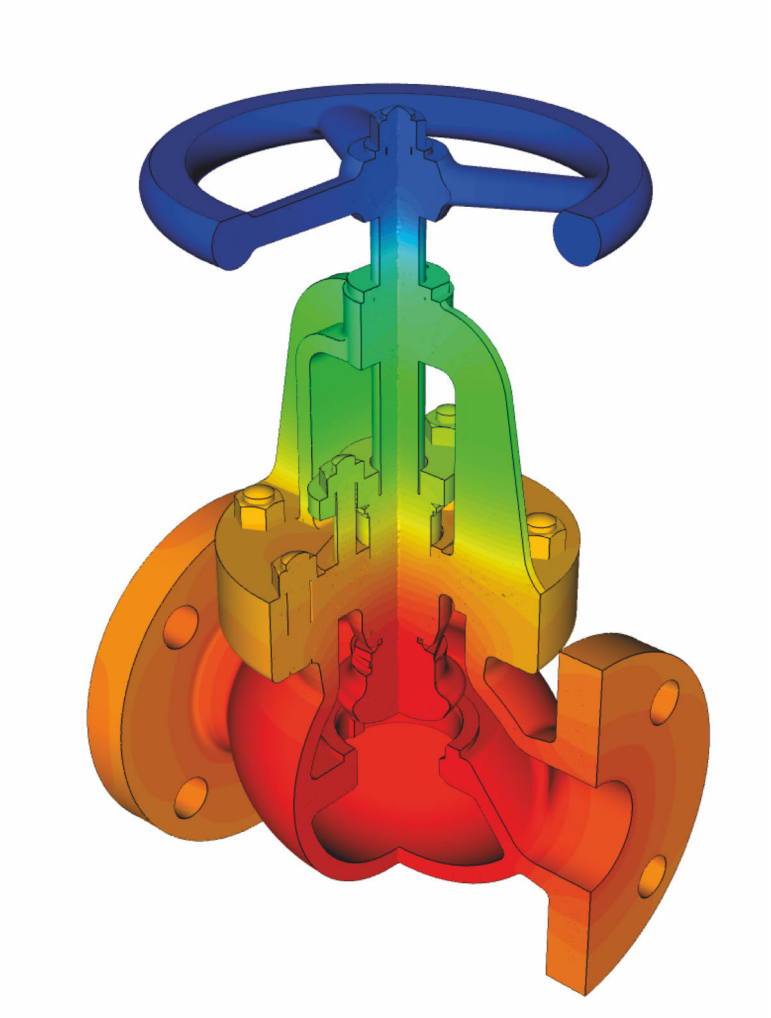
Parallel Algorithms Research Laboratory

Significant events

- M. Jaroš was awarded the Best Student Research Presentation Prize at the International Conference on Computer Graphics and Digital Image Processing (CGDIP 2017).
- The “BEM4I: A massively parallel boundary element solver” poster by J. Zapletal, M. Kravčenko, M. Merta, and L. Malý ranked among the first nine nominated posters for the Best Poster Award at the SC17 conference. (A total of 169 poster contributions were sent to the poster section of the conference with 98 being accepted for presentation).
- The ESPRESO solver for solving structural mechanics problems was nominated for the Innovation Radar Prize 2017 of the European Commission.
- J. Zapletal, a researcher at IT4Innovations and graduate at the Faculty of Electrical Engineering and Computer Science at VŠB – Technical University of Ostrava won the first place in the Joseph Fourier Prize competition for the best research within PhD studies in the field of computer science and computational sciences. He was also awarded the Prof. Babuska Prize for Computational Sciences.

Selected publications

- R. Halama, A. Markopoulos, R. Jančo, M. Barteckỳ: Implementation of MAKOC Cyclic Plasticity Model with Memory. Advances in Engineering Software (2017). DOI: 10.1016/j.advengsoft.2016.10.009. IF=3; Q1.
- M. Merta, L. Říha, O. Meca, A. Markopoulos, T. Brzobohatý, T. Kozubek, V. Vondrák: Intel Xeon Phi acceleration of hybrid total FETI solver. Advances in Engineering Software (2017). DOI: 10.1016/j.advengsoft.2017.05.001. IF=3; Q1.
- I. Janeček, P. Naar, M. Stachoň, F. X. Gadéa, R. Kalus: Fragmentation of KrN clusters after electron-impact ionization I: Short-time dynamics and multiscale treatment. Physical Chemistry Chemical Physics (2017). DOI: 10.1039/C6CP07479K. IF=4,449; Q1.
- I. Janeček, M. Stachoň, F. X. Gadéa, R. Kalus: Fragmentation of KrN clusters after electron-impact ionization II: Long-time dynamics of Kr7+ evolution and the role of initial electronic excitation. Physical Chemistry Chemical Physics (2017). DOI: 10.1039/C7CP03940A. IF=4,449; Q1.
- J. Zapoměl, P. Ferfecki, J. Kozánek: Modelling of magnetorheological squeeze film dampers for vibration suppression of rigid rotors. International Journal of Mechanical Sciences (2017). DOI: 10.1016/j.ijmecsci.2016.11.009. IF=2,884; Q1.



Thermal calculation of the valve using
the open-source ESPRESO package

Advanced Data Analysis and Simulations Laboratory

Significant events

- The HyperLoom platform was released as open source software under the modified BSD licence. http://hyperloom.eu The poster titled "How To Do Machine Learning on Big Clusters" dedicated to HyperLoom was selected among the nine best posters at the international SC17 conference.
- The review of the Urban Thematic Exploitation Platform within the contract research funded by ESA was successfully defended. A successor project is in preparation for further funding of the platform in order to ensure its sustainability.
- The software package for RQA analysis and time series prediction based on the theory of chaos was developed and published (authors T. Martinovič and G. Zitzlsberger). https://code.it4i.cz/ADAS/RQA_HPC
- The IT4S1 system for automatized monitoring of terrain motions and infrastructure via the satellite Sentinel-1 system by radar interferometry method was developed (author Milan Lazecký).
- Grakova E., J. Hanzelka a J. Křenek collaborated with the OZO Ostrava company in development of the GAIA software (https://gaia.iti.cz), which enables us to monitor, in real time, the level to which the city waste receptacles are filled using sensors attached to them. To design and optimize the waste collection routes, a metaheuristic algorithm was adopted and connected to the user interface.

Selected publications

- Režnar, T., Martinovič, J., Slaninová, K., Grakova, E., Vondrák, V. Probabilistic time-dependent vehicle routing problem. Central European Journal of Operations Research (2017). DOI: 10.1007/s10100-016-0459-2. IF=0,659; Q4.
- Drwięga, T., Lampart, M., Oprocha, P. Limit Sets, Attractors and Chaos. Qualitative Theory of Dynamical Systems (2017). DOI: 10.1007/s12346-015-0163-y. IF=0,825; Q2.
- Svoboda, Z., Bizovska, L., Janura, M., Kuboňová, E., Janurová, K., Vuillerme, N. Variability of spatial temporal gait parameters and center of pressure displacements during gait in elderly fallers and nonfallers: A 6-month prospective study. PLoS ONE (2017). DOI: 10.1371/journal.pone.0171997. IF=2,806; Q1.
- Theuer, M., Vavřík, R., Vondrák, V., Kuchař, S., Šír, B., Portero, A.: Efficient methods of automatic calibration for rainfall-runoff modelling in the Floreon+ system. Neural Network World (2017). DOI: 10.14311/NNW.2017.27.022. IF=0,394; Q4.

The Advanced Data Analysis and Simulations laboratory provides support for deploying new tools to enable easy and efficient use of IT4Innovations infrastructure for machine learning tasks. The laboratory is actively involved in the development of new machine learning applications that allow modeling of complex systems using regression, classification and clustering methods. The laboratory also develops tools to verify the accuracy of these models. In collaboration with the pharmaceutical industry, the laboratory develops predictive models used for new drug design by means of deep learning as well as traditional statistical methods.

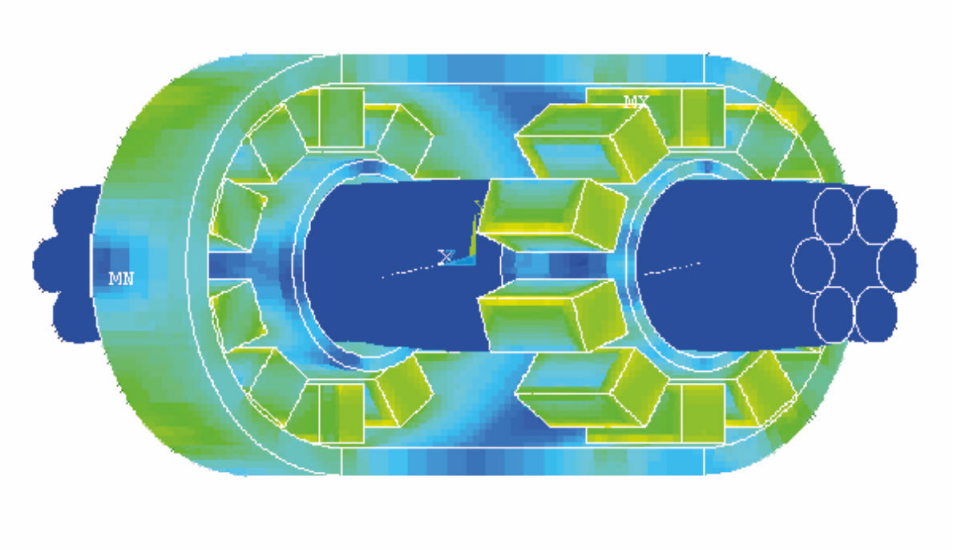
Modelling for Nanotechnologies Laboratory

Significant events

- On 24th November 2017, Ing. Zuzana Mrázková successfully defended her PhD thesis before a Czech – French committee.
- In June 2017, Ing. Jan Chochol successfully defended his PhD thesis before a Canadian – Czech committee.

Selected publications

- Tian H., Z. W. Seh, K. Yan, Z. Fu, P. Tang, Y. Lu, R. Zhang, D. Legut, Y. Cui, Q. Zhang: Theoretical Investigation of Two-Dimensional Layered Materials as Protective Films for Lithium and Sodium Metal Anodes. Advanced Energy Materials (2017). DOI: 10.1002/aenm.201602528. IF=16,5; Q1.
- Zhang H., Z. Fu, R. Zhang, Q. Zhang, H. Tian, D. Legut, T. C. Germannd, Y. Guoa, S. Due, and J. S. Francisco: Designing flexible 2D transition metal carbides with strain-controllable lithium storage. Proceedings of the National Academy of Sciences (2017). DOI: 10.1073/pnas.1717219115. IF=10,4; Q1.
- Ma Y., Y. Alattar, J. Zhou, M. Eldlio, H. Maeda, J. Pištora, M. Čada: Semiconductor-based plasmonic interferometers for ultrasensitive sensing in a terahertz regime. Optics Letters (2017). DOI: 10.1364/OL.42.002338. IF = 3,416; Q1.
- Mrázková Z., M. Foldyna, S. Misra, M. Al-Ghzaiwat, K. Postava, J. Pištora, P. R. I.Cabarrocas: In-situ Mueller matrix ellipsometry of silicon nanowires grown by plasma-enhanced vapor-liquid-solid method for radial junction solar cells. Applied Surface Science (2017). DOI: 10.1016/j.apsusc.2016.12.199. IF = 3,387; Q1.
- Chochol J., K. Postava, M. Čada, J. Pištora: Experimental demonstration of magneto-plasmon polariton at InSb(InAs)/dielectric interface for terahertz sensor application. Scientific Reports (2017). DOI: 10.1038/s41598-017-13394-0. IF = 4,259; Q1.



Magnetizing head of the defectoscope – distribution of permanent magnets

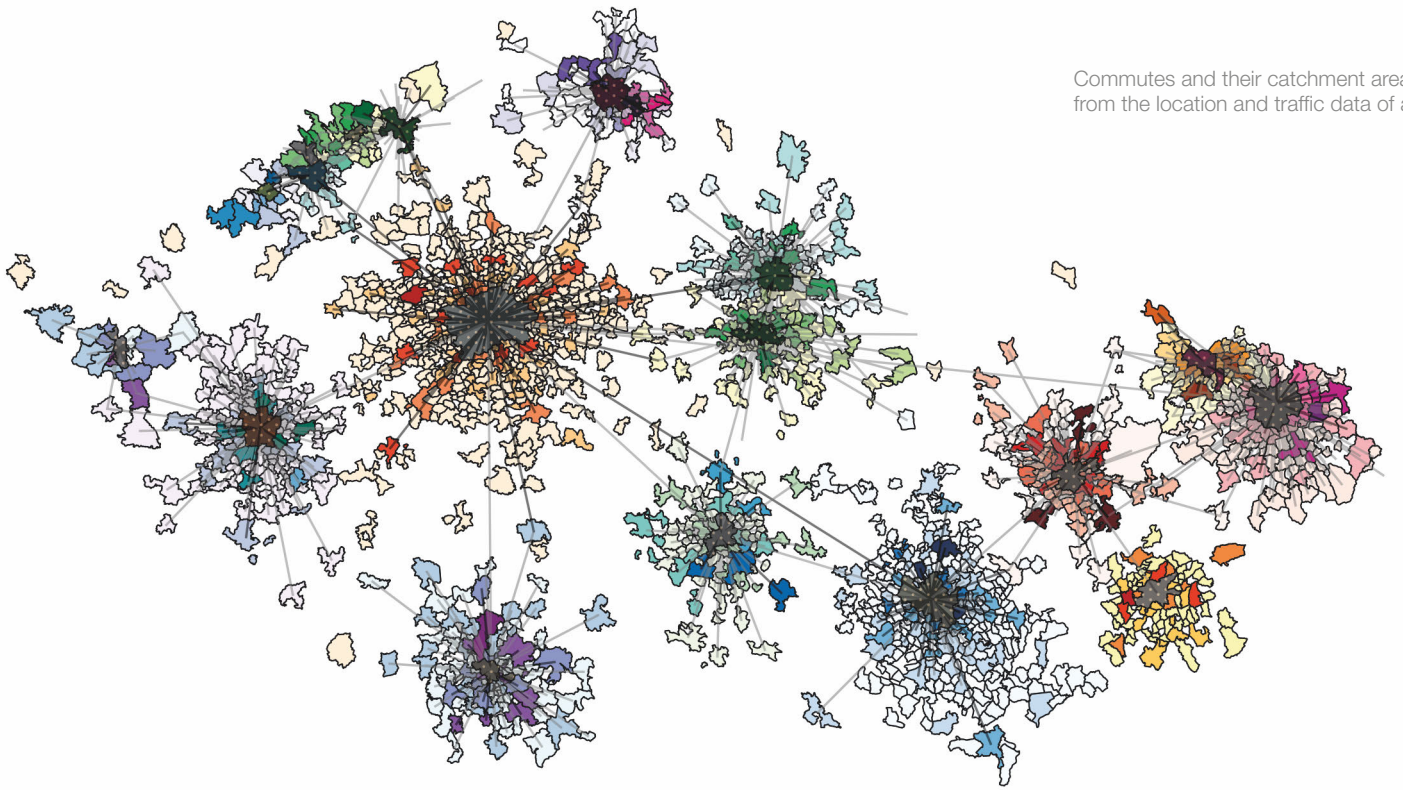
Big Data Analysis Laboratory

Significant events

- Dr. Ing. Martin Hasal won the second place in the Prof. Babuška Prize competition organized by the Czech Society of Mechanics and the Union of Czech Mathematicians and Physicists since 1994.
- In 2017, the prestigious “Artificial Inteligence and Reasoning” project within the “Excellent Research Teams” Call announced by OP RDE was initiated by IT4Innovations in partnership with the Czech Technical University in Prague, and the University of West Bohemia in Pilsen.
- The “Security of mobile devices and communication” project, supported by the Technology Agency of the Czech Republic, no. TF01000091, where part of the laboratory staff participated, was concluded successfully.

Selected publications

- Venskus J., Treigys P., Bernatavičiene J., Medvedev V., Vozňák M., Kurmis M., Bulbenkiene, V. Integration of a Self-Organizing Map and a Virtual Pheromone for Real-Time Abnormal Movement Detection in Marine Traffic. Informatica (2017). DOI: 10.15388/Informatica.2017.133. IF=1,056; Q2
- Továrek J., Partila P. Speaker identification for the improvement of the security communication between law enforcement units. Proceedings of SPIE - The International Society for Optical Engineering (2017). DOI: 10.1117/12.2261796.



Commutes and their catchment areas, processed
from the location and traffic data of a mobile network

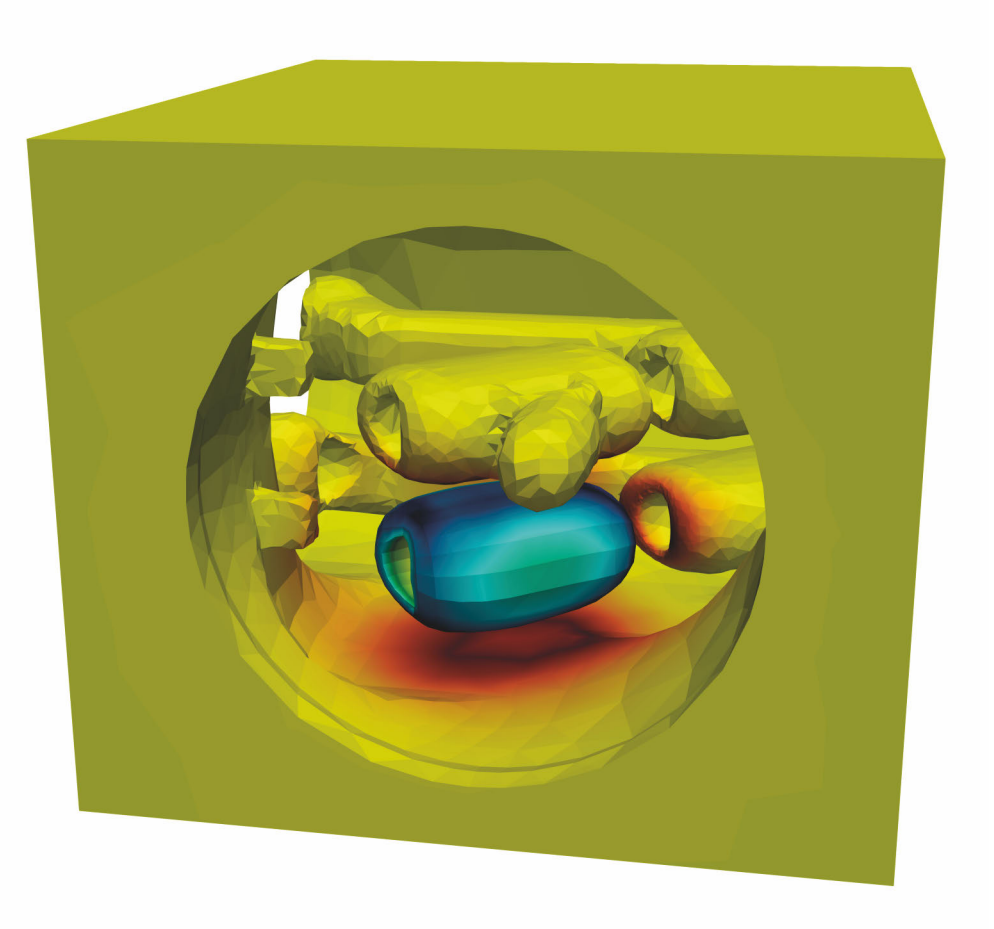
Infrastructure Research Laboratory

Significant events

- A new PermonQP package was released, and the PermonSVM package was published. http://permon.it4i.cz
- In September 2017, the PermonSVM and PermonQP software packages were published on the PETSc website. https://www.mcs.anl.gov/petsc/
- The PERMON poster by M. Čermák, V. Hapla, D. Horák, J. Kružík, M. Pecha, R. Sojka, J. Tomčala won the Best Poster Award at the HPCSE 2017 conference.
- J. Kružík won the opportunity to participate at the prestigious summer school within the Argonne Training Program on Extreme-Scale Computing (30th July – 11th August 2017, St. Charles, Illinois, USA).

Selected publications

- Čermák M., V. Hapla, J. Kružík, A. Markopoulos, A. Vašatová: Comparison of different FETI preconditioners for elastoplasticity. Computers & Mathematics with Applications (2017). DOI: 10.1016/j.camwa.2017.01.003. IF 1,531; Q1.
- Sysala S., M. Čermák, T. Ligurský: Subdifferential-based implicit return-mapping operators in Mohr-Coulomb plasticity. ZAMM Zeitschrift fur Angewandte Mathematik und Mechanik (2017). DOI: 10.1002/zamm.201600215. IF 1,332; Q2.
- Horák D., V. Hapla, J. Kružík, R. Sojka, M. Čermák, J. Tomčala, M. Pecha, Z. Dostál: A note on massively parallel implementation of feti for the solution of contact problems. Advances in Electrical and Electronic Engineering (2017). DOI: 10.15598/aeee.v15i2.2322.
- Horák D., Z. Dostál, V. Hapla, J. Kružík, R. Sojka, M. Čermák: Projector-less TFETI for contact problems: Preliminary results. Civil-Comp Proceedings 111 (2017). DOI: 10.4203/ccp.111.8.



Electric intensity on an electrode optimized
by multiresolution approach based on subdivision
surfaces and the boundary element method.
(Due to restructuring at IT4Innovations,
the BEM4I development team joined
the Infrastructure Research Laboratory
at the beginning of 2018.)

Projects

NATIONAL GRANTS

IT4Innovations excellence in science (2016–2020)

Project ID: LQ1602
Principal investigator for 2017: Dr. Ing. Martin Palkovič
(from 1st January 2018 Prof. Dr. Ing. Tomáš Kozubek)

In the years 2011 to 2015, the IT4Innovations Centre of Excellence project was jointly implemented by the following partners: VŠB – Technical University of Ostrava, the University of Ostrava, the Silesian University in Opava, Brno Technical University, and the Institute of Geonics of the Czech Academy of Sciences. The cooperation of these institutions is currently continuing within the National Programme of Sustainability II (IT4Innovations excellence in science) by conducting excellent research in the fields of high performance computing and cyberphysical systems.

Complex study of effects in low-dimensional quantum spin systems (2017–2018)

Project ID: 8X17046
Principal investigator: Dr. Ing. Dominik Legut

The project aims to investigate the characteristics of the selected two-dimensional magnetically-frustrated quantum system $Cu(tn)Cl_2$(tn=1.3–diaminopropan = $C_3H_{10}N_2$) from the first principles, with the goal of contributing to the understanding of the origin of the unconventional phenomena observed in two-dimensional frustrated magnets.

THE MINISTRY OF EDUCATION, YOUTH AND SPORTS GRANTS FOR SPECIFIC UNIVERSITY RESEARCH (2017)

Creation of rendering service

Project ID: SP2017/107
Principal investigator: Dr. Ing. Tomáš Karásek

The objective of this project was to extend the existing possibilities of the IT4Innovations large infrastructure with an opportunity to provide rendering as a service for external users of this infrastructure. The project was implemented with the non-profit organization Blender Institute, Amsterdam.

Terahertz spectroscopy of photonic structures using advanced materials

Project ID: SP2017/154
Principal investigator: Ing. Martin Mičica

This project aimed to investigate the use of advanced materials – molecular crystals, molecular gases, hexaferrites, III-V semiconductors, and thermoplastics, and their use in construction of sources, insulators, sensors, and other photonic structures for terahertz applications.

Massively parallel modelling of strongly nonlinear processes in mechanics

Project ID: SP2017/156
Principal investigator: Prof. Dr. Ing. Petr Horyl

All topics elaborated in the project aimed to solve current and very challenging, strongly nonlinear practical problems in engineering. The objective was to increase the present value of either new or innovative products. The newly proposed solution is based on finer discretizations of given structures in order to ensure results that are more reliable.

Efficient implementation of the boundary element method III

Project ID: SP2017/165
Principal investigator: Dr. Ing. Michal Merta

This was a successor project of the SGS SP2016/113 and SP2015/160 projects, and its objective was to further develop the existing BEM4I library of parallel solvers based on the boundary element method.

Numerical methods for modelling environmental processes

Project ID: SP2017/167
Principal investigator: Dr. Ing. Tomáš Brzobohatý

The project aimed to interconnect several scientific domains having a direct connection to numerical solution of problems associated with prediction of risks such as emission of hazardous substances, spread of air pollution, and exposure of the population to environmental hazards such as floods.

Modelling of collision processes in low-temperature plasma

Project ID: SP2017/168
Principal investigator: Doc. Dr. RNDr. René Kalus

The project aimed to support student dissertation projects in the field of numerical modelling of collision processes in low-temperature noble gas-based plasma.

PERMON toolbox development III

Project ID: SP2017/169
Principal investigator: Doc. Dr. Ing. David Horák

This project aimed to further develop the PERMON toolbox using the state-of-the-art theoretical knowledge in the field of discretization techniques, quadratic programming algorithms, and domain decomposition methods.

Optimization of machine learning algorithms for an HPC platform

Project ID: SP2017/177
Principal investigator: Dr. Ing. Kateřina Slaninová

The project focused on the use of algorithms of unsupervised machine learning for preprocessing the data for supervised machine learning algorithms. Such preprocessed data can lead to increasing convergence of the given methods and making the outcome resulting thereof more precise.

Solution of graph problems on uncertainty time-space graphs using HPC

Project ID: SP2017/182
Principal investigator: Dr. Ing. Jan Martinovič

The objective of the project was to develop algorithms allowing effective calculations of given characteristics of extensive dynamic uncertainty graphs, and analysis of these algorithms using the dynamic systems development methods.

Thermal expansion of Fe-Ti alloys

Project ID: SP2017/184
Principal investigator: Dr. Ing. Dominik Legut

Within the project, investigation of the mechanism responsible for reduction or total suppression of thermal expansion of two-phase titanium alloys exhibiting magnetostriction was conducted both theoretically and experimentally. The main objective of the project was to find the most suitable method for suppressing the above-mentioned phenomena.

PROJECTS SUPPORTED BY THE GRANT AGENCY OF THE CZECH REPUBLIC

New nonlinear and magneto-optical phenomena in periodic structures (2015–2017)

Project ID: GA15-08971S
Principal investigator: Doc. Dr. Mgr. Kamil Postava
Within the project, generation of quantum-correlated photon pairs in modern photonic structures was studied, especially in non-linear thin-film metal-dielectric structures, in magneto-optical periodic structures, and periodically-polar structures.

Efficient lifetime estimation techniques for general multiaxial loading (2015–2017)

Project ID: GA15-18274S
Principal investigator: Doc. Dr. Ing. David Horák

The project was focused on methods for predicting fatigue life for multiaxial loading in the field of low-cycle fatigue, i.e. in cases where plasticity cannot be neglected. In order to achieve a high-quality result of complex calculations in an acceptable timeframe and allow adequate time to evaluate them, the core of the PragTic fatigue solver used for all fatigue analyses was converted into a fully parallel scalable application.

Novel fuel materials for Generation IV nuclear reactors (2017–2019)
Project ID: GA17-27790S
Principal investigator: Dr. Ing. Dominik Legut

The project is attempting to build an understanding of mechanical and thermodynamic properties of alloys designated for nuclear fuel for Generation IV nuclear reactors, alloys containing f-electrons, namely carbides and uranium, thorium, and plutonium tetrafluorides. Based on the ab-initio electronic structure calculations, magnetic, elastic, dynamic (phonons), and thermodynamic behaviour will be determined in (U/Th/Pu)-C systems. The main objective is to explain thermal expansion of actinide carbides, and especially negative thermal expansion observed in UC2 at atomic level.

PROJECTS SUPPORTED BY THE TECHNOLOGY AGENCY OF THE CZECH REPUBLIC

Transport Systems Development Centre (2017–2019)
Project ID: Te01020155
(project supported by the Centre of Competence programme)
Principal investigator: Prof. Dr. Ing. Ivo Vondrák

The Transport Systems Development Centre was based on the long-term partnership between research and private companies determining the direction of intelligent mobility development in the Czech Republic. We have jointly decided to face the challenge ofa continuous search for balance between the need for movement of modern society and the negative impacts of mobility. We relied on experienced teams, excellent knowledge of the environment, willingness to cooperate and the shareing of risks associated with setting the trends in the area of mobility control corresponding to the needs in the 21st century.

Centre of Competence for Molecular Diagnostics and Personalized Medicine (2014–2019)
Project ID: Te02000058
(project supported by the Centre of Competence programme)
Principal investigator for 2017: Dr. Ing. Martin Palkovič
(from 1st January 2018 Dr. Mgr. Branislav Jansík)

The primary objective of the project is to apply and further foster the existing expert experience and achieve a critical mass of participants and knowledge in research, development, manufacturing, protection of Intelectual Property, certification, technology transfer, and commercionalization of in vitro diagnostics, in order to create a market-oriented flexible national network of important institutions in the area of biomarkers and molecular diagnostics.

Parallelized Reaction-Transport Model of Contamination Spread in Groundwater (2017–2019)
Project ID: Th02030840
(project supported by the EPSILON programme for the support of applied research and experimental development)
Investigator for IT4Innovations: Dr. Ing. Michal Podhorányi

The objective of the project is to improve the possibilities of a potential risk analysis of environmental contamination due to the long-term radioactive substances spread around a deep radioactive waste repository via the surrounding rocky environment.

PROJECT OF OPERATIONAL PROGRAMME RESEARCH, DEVELOPMENT AND EDUCATION

IT4Innovations National Supercomputing Center – Path to Exascale (2017–2021)
Project ID: EF16_013/0001791
Principal Investigator: Dr. Mgr. Branislav Jansík

Some objectives of the project are to extend IT4Innovations in-house research in the field of modelling photonic and spin-photonic structures, design of progressive materials based on electronic structure calculations, and bioimage analysis using HPC. For the IT4Innovations infrastructure, in-house research is an important source of HPC expertise, which is reflected in services provided by this infrastructure to its users.

INTERNATIONAL GRANTS

ANTAREX – AutoTuning and Adaptivity appRoach for Energy efficient eXascale HPC systems (2015–2018)
Project ID: 671623
(H2020-FETHPC-2014 Call)
Principal Investigator: Dr. Ing. Jan Martinovič

The main goal of the ANTAREX project is to design a self-adaptive approach for applications run on supercomputers using a Domain Specific Language. Management their runtime and implementation of auto-tunning will enable us to achieve energy-efficient heterogenous HPC systems on the exascale level.
ww.antarex-project.eu

ExCAPE – Exascale Compound Activity Prediction Engine (2015–2018)
Project ID: 671555
(H2020-FETHPC-2014 Call)
Principal Investigator: Dr. Ing. Jan Martinovič

Within this project, IT4Innovations is involved in development of state-of-the-art scalable algorithms and their implementations suitable for running on future Exascale machines. The relevant algorithms are developed for solving complex problems in the field of pharmacology with respect to the necessity of processing large data sets essential for industrial drug design.
www.excape-h2020.eu

READEX – Runtime Exploitation of Application Dynamism for Energy-efficient eXascale computing (2015–2018)
Project ID: 671657
(H2020-FETHPC-2014 Call)
Principal Investigator: Dr. Ing. Lubomír Říha

The role of IT4I in this project is evaluation of dynamism in HPC applications, their manual tuning, and evaluation and validation of the developed tool to optimize power consumption, taking the results of manual tuning as the baseline.
www.readex.eu

LOWBRASYS – A Low Environemntal Impact Brake System (2017–2018)
Project ID: 636592
(H2020-MG-2014_TwoStages Call)
Principal Investigator: Doc. Dr. Mgr. Jana Kukutschová

Within this project, a new generation of innovative technologies for cleaner and more efficient road transport and improving air quality with positive effects on both environment and human life will be developed. The project also responds to the requirement to comply with stricter legal regulations for emissions and air quality in the European Union in the future.
www.lowbrasys.eu

EXPERTISE – Models, Experiments and High Performance Computing for Turbine Mechanical Integrity and Structural Dynamics in Europe (2017–2021)
Project ID: 721865
(H2020-MSCA-ITN-2016 Call)
Principal Investigator: Prof. Dr. Ing. Tomáš Kozubek

The objective of this four-year long project is to educate researchers able to participate in interdisciplinary cooperation. The collaboration between industrial partners and research organizations will speed up development of key technologies for the development of turbines and their rapid commissioning in practice.
www.msca-expertise.eu

TETRAMAX – Technology transfer via multinational application experiments (2017–2021)
Project ID: 761349
(H2020-ICT-2016-2 Call)
Principal Investigator: Dr. Ing. Martin Palkovič

Within this project, the "Smart Anything Everywhere" initiative will be implemented in the field of Customized Low Energy Computing for cyberphysical systems and the Internet of Things. The key purpose of this initiative is to accelerate innovations in European industry. The initiative connects technical and application knowledge and experience, which helps small and medium-sized enterprises adopt advanced digital technologies more effectively and efficiently.
www.tetramax.eu

CloudiFacturing – Cloudification of Production Engineering for Predictive Digital Manufacturing (2017–2021)
Project ID: 768892
(H2020-FOF-2017 Call)
Principal investigator: Dr. Ing. Tomáš Karásek

The mission of the project is to contribute to efficient use of high performance computing by European small and medium-sized production companies and thus increase their competitiveness. This projects aims at optimization of production processes and productivity of companies using HPC-based modelling and simulation as well as cloud services.
www.cloudifacturing.eu

PROJECT OF THE EUROPEAN SPACE AGENCY

Urban TEP – Urban Thematic Exploitation Platform (2015–2018)
Principal investigator: Doc. Dr. Mgr. Vít Vondrák

The main objective of this project is to implement a software platform which will help solve not only the key research questions but also social challenges arising from the global phenomenon of urbanisation. The main role of IT4Innovations in this project is to provide state-of-the-art technologies and expert knowledge in the field of High Performance Computing. IT4Innovations offers services in the form of processing and storing the data, which are essential for access, analysis, and visualization of geospatial data and derived products.
https://urban-tep.eo.esa.int

OTHER PROJECTS

IPCC – Intel® Parallel Computing Center at IT4Innovations National Supercomputing Center (2015–2017)
Principal investigator: Doc. Dr. Mgr. Vít Vondrák

In 2015, IT4Innovations was included in the Intel® Parallel Computing Center programme. For two years, this grant funded the research of a group of scientists engaged in the development of algorithms and libraries for highly parallel computing systems. Algorithms were also optimized for the latest supercomputer technologies developed by Intel.
www.ipcc.it4i.cz

Collaboration with the commercial sector

Collaboration with the commercial sector is implemented at IT4Innovations mainly in the form of contract research.

Our contract research in 2017 included collaboration with ten companies, one university, and one hospital:

- K2 atmitec s.r.o.
- FERRAM STROJÍRNA, s.r.o.
- Continental Automotive Czech Republic s.r.o.
- University of Ostrava
- University Hospital Ostrava
- Invent Medical Group, s.r.o.
- ING corporation, spol. s.r.o.
- Zdravotní a sociální služby s.r.o.
- PTS Josef Solnař, s.r.o.
- BORCAD cz s.r.o.
- VAKAR s.r.o.
- ITA s.r.o.

We have cooperated with the ING Corporation in developing cranial remodelling ortheses (helmets), which are used to correct asymmetric growth of the heads of children.

EDUCATIONAL AND TRAINING ACTIVITIES

EDUCATIONAL AND TRAINING ACTIVITIES

Computational Sciences PhD study programme

Since 2015 IT4Innovations has been involved in the realization of the doctoral study program Computational Sciences. Students focus on the use of HPC and HPDA in both science and industry. Altogether twenty-one students were enrolled in the Computational Sciences PhD study programme at the end of 2017.

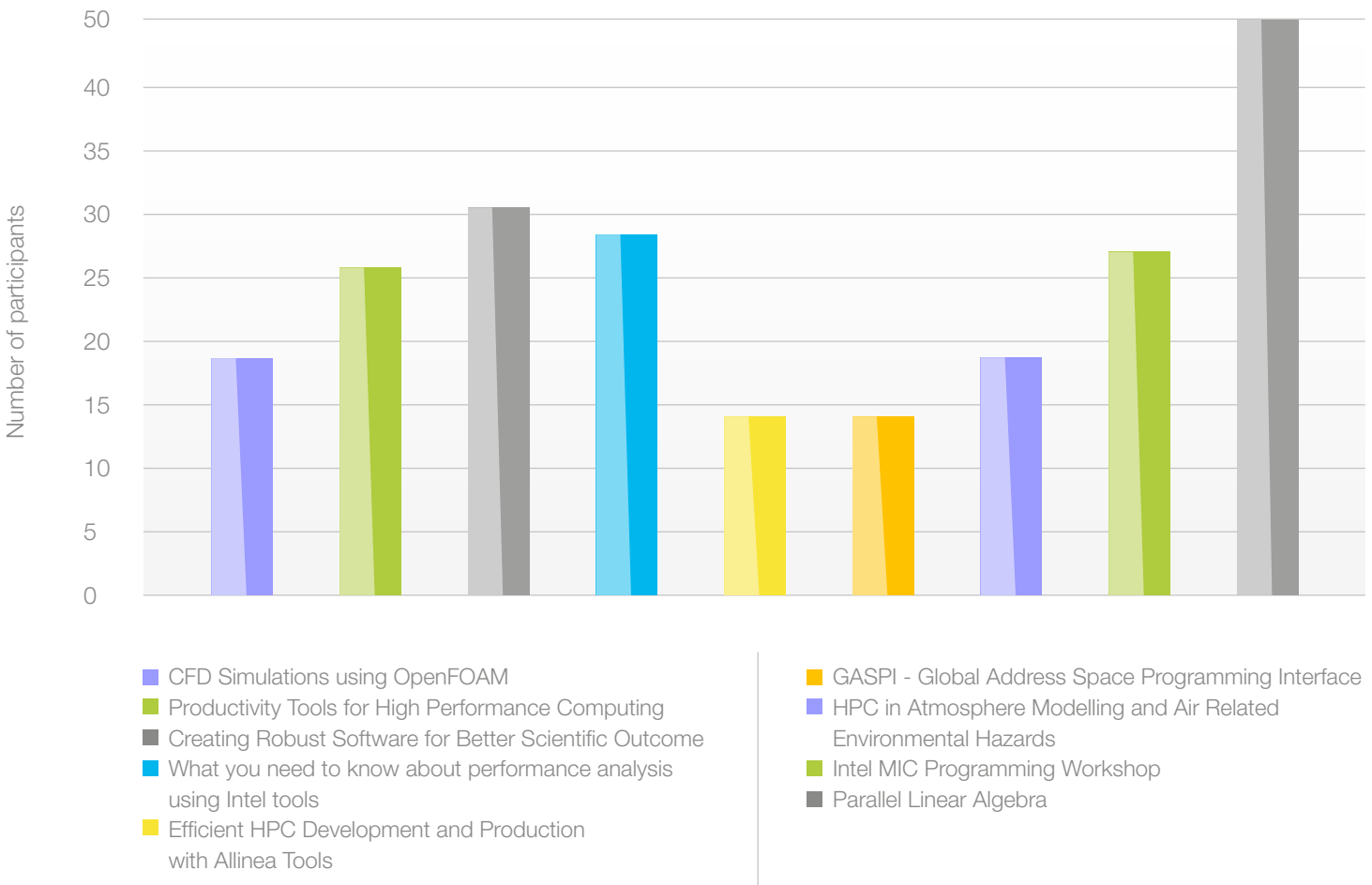
Training activities

IT4Innovations supports the scientific community and its users by offering high-quality courses, workshops, and other training activities. The primary objective of these activities is to broadly increase competency of users to efficiently utilize the unique computing infrastructure of IT4Innovations. In the broader sense, we also aim to raise awareness and knowledge in the field of HPC nationwide in both academia as well as the commercial sector.

The topics of the courses offered by IT4Innovations are focused on computer systems and architectures, programming techniques, tools, libraries, and applications. In 2017, nine training events were held with a total of 227 participants. We would like to highlight the most significant events led by renowned foreign experts as follows:

- **Parallel Linear Algebra** workshop (Mathieu Faverge, Florent Pruvost, Gilles Marait from Bordeaux INP, Zdeněk Strakoš from Charles University) focused on modern parallel methods for solving large linear systems of equations using parallel computers;
- Two-day course on **Global Address Space Programming Interface** (Christian Simmendinger, T-Systems Solutions for Research GmbH), who presented an asynchronous dataflow programming model for PGAS as an alternative to MPI programming;
- **Efficient HPC Development and Production with Allinea Tools** course (Florent Lebeau, ARM, UK) focused on the use of Allinea company tools on the Salomon supercomputer;
- Two-day **Creating Robust Software for Better Scientific Outcome** workshop (Anshu Dubey and Rinku Gupta, Argonne National Laboratory, USA) focused on well-tested techniques in the field of software engineering, which are explicitely adjusted to suit the needs of computational sciences and engineering.

Training activities in 2017



In 2017, we were awarded the status of PRACE Training Centre. We believe that the PRACE Panel of Experts were captivated by the creditable educational history of our centre. It comprises an average of 10 courses, 16 lecture days, and 255 participants per each academic year. Moreover, it is unique, with a balance between the local junior as well as renowned external lecturers, organization of several large international training events (e.g. PRACE seasonal schools), collaboration with PATC (PRACE Advanced Training Centre) including hosting their courses, and among others, a convenient geographical location near the three borders of the Czech and Slovak Republics and Poland. Naturally however, the most important aspect was the portfolio of specialized courses led by our colleagues for the PRACE initiative. In 2017, we organized two PTC courses led by our colleagues: Productivity Tools for High Performance Computing (Branislav Jansík, David Hrbáč, Josef Hrabal, Lukáš Krupčík, Lubomír Prda, and Roman Slíva) and CFD Simulations Using OpenFOAM (Tomáš Brzobohatý). In 2018, courses focused on Intel Xeon Phi Programming and The Portable Extensible Toolkit for Scientific Computing are planned. These topics are quite rare in the existing PATC portfolio, which highlights the contribution of IT4Innovations to the PRACE training programme.

Photos from courses at IT4Innovations in 2017

PRACE Summer of HPC training week at IT4Innovations, July 2017

Trip to Dolní Vítkovice, July 2017

PRACE Summer of HPC 2017: Shukai Wang, Imperial College London graduate, worked at IT4Innovations on the project Performance Visualization for Bioinformatics Pipelines (mentor Dr. Ing. Jan Martinovič)

2017 was the fifth consecutive year that the Partnership for Advanced Computing in Europe (PRACE) has enabled 21 students to do an international summer internship with one of the participating supercomputing centres throughout Europe. Annually, the programme starts with a joint kick-off HPC basics training week. Held this year in Ostrava, the Czech Republic, the training course was led by lecturers from IT4Innovations and one lecturer from the partner centre of SurfSARA from the Netherlands. During that week, students were introduced to the programme objectives as well as HPC basics. They also had an opportunity to visit interesting local sites.

Projects of Operational Programme Research, Development, and Education

Technique for the Future (2016–2020)
Project ID: CZ.02.2.69/0.0/0.0/16_015/0002338
(02_16_015 Call)
IT4Innovations Project Specialist: Doc. Dr. RNDr. René Kalus

The project of the VŠB – Technical University of Ostrava „Technique for the Future“ aims at creating or modifying strategic study programmes so that they reflect the demands of employers and prepare students for successful entry into the labor market. The project focuses on the introduction of progressive teaching methods using state-of-the-art technical equipment, collaboration with companies and graduates, strengthening the internationalism of the university, improving work with students with various handicaps, improving the quality system and management of the university, and promoting student entrepreneurship.

Doctoral School for Education in Mathematical Methods and Tools in HPC (2017–2022)
Project ID: CZ.02.2.69/0.0/0.0/16_018/0002713
(02_16_018 Call)
Principal Investigator: Prof. Dr. Ing. Tomáš Kozubek

The main objective of the project is to establish the Doctoral School for Education in Mathematical Methods and Tools in HPC integrating doctoral studies at Charles University, Czech Academy of Sciences, and VŠB-TUO. Part of the project is to modernize and internationalize one of the doctoral programs of the school (Computational Sciences, VŠB-TUO) as well as to create new double degree programs (planned in collaboration with Università della Svizzera italiana, Lugano, Switzerland, and Université Toulouse III Paul Sabatier, France). The project builds on the related ERDF IT4Innovations Educational Training Center project. Both projects are implemented with the support of European funds.

IT4Innovations Educational Training Center (2017–2022)

Project ID: CZ.02.1.01/0.0/0.0/16_017/0002628
(02_16_017 Call)
Principal Investigator Ing. Radim Mrázek

The implementation of the project will lead to the establishment of a training infrastructure to support research-oriented programmes focused on the use of high performance computing technologies (HPC). In the wider context, the project objective is to eliminate the barrier blocking a higher rate of HPC technology exploitation under the conditions of the Czech Republic. It consists mainly of a lack of specialists and experts in High Performance Computing (HPC).

The projected built area of the new training centre will be 674 m^2. In the building, there will be an auditorium with a capacity of 150 people, a computer room with a capacity of 25 people, and 2 combined lecture rooms with a total capacity of 50 people. The overall capacity of the centre will thus be 225 students. The lecture areas will be equipped with the modern information and audiovisual technology essential for studies within the study programmes oriented towards exploitation of high performance computing technologies.

The building will meet the current technical requirements for efficient and safe operation, and above all, it will be equipped with two heat sources. Taking advantage from its location in the vicinity of the IT4Innovations infrastructure, the building will use the residual heat generated by the supercomputers in the IT4Innovations building. This will make the building more environmentally-friendly.

Visualization of the IT4Innovations Educational Training Center

IT4Innovations
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supercomputing
center@#01%101

www.it4i.cz

Postal address
VŠB – Technical University of Ostrava
17. listopadu 15
708 33 Ostrava – Poruba
Czech Republic

E-mail: info@it4i.cz
Phone: +420 597 329 602

Location
VŠB – Technical University Of Ostrava
Studentská 6231/1B
708 33 Ostrava – Poruba
Czech Republic

MINISTRY OF EDUCATION,
YOUTH AND SPORTS

This publication was supported by The Ministry of Education, Youth and Sports from the Large Infrastructures for Research, Experimental Development and Innovations project „IT4Innovations National Supercomputing Center – LM2015070"

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