

IT4INNOVATIONS REVIEW 2016

IT4Innovations
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MINISTRY OF EDUCATION,
YOUTH AND SPORTS

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IT4INNOVATIONS REVIEW 2016

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Dear readers,

In this review of 2016, we would like to introduce you to the most important events of the previous year, to the financial management of IT4Innovations, to the use of super-computing services, and to the research we have been working on.

The year 2016 was the first year of sustainability for the 'Center of Excellence IT4Innovations' project, implemented in 2011-2015 within the Operational Programme Research and Development for Innovation, which allowed the foundation of our centre. Several national and international grants helped us to secure the running of our centre last year. The most important one is the grant from the Ministry of Education, Youth and Sports of the Czech Republic (MEYS), IT4Innovations National Supercomputing Center, supported by funds dedicated to large infrastructures for research, experimental development, and innovation. Thanks to this grant, we continue to provide open access to the most powerful and state-of-the-art supercomputer systems in the Czech Republic. In the framework of the National Sustainability Programme II project (also from the MEYS), IT4Innovations Excellence in Science, we continue to carry out excellent research in the area of supercomputing and embedded systems, together with our partners.

We managed to enhance our status within the international HPC community several times in 2016. We co-organized two major conferences in Prague, HiPEAC 2016 in January and PRACEdays 2016 in May. In March, we had the opportunity to welcome the Intel Xeon Phi Users Group in Ostrava. In July, we became a member of the European Technology Platform for HPC and consolidated our position in the European research area.

In 2016 we organized three open access competitions through which we divided the maximum possible computational capacity of our supercomputers. The demand for computing time in those competitions exceeded our supply. Through contract research, we have further developed cooperation with, and support for industrial partners. The three international projects (funded from the Seventh Framework Programme of the European Union) we have been involved with were concluded in 2016, with excellent evaluations. Concurrently, we have successfully continued with our international projects funded from the Horizon 2020 Programme of the European Union.

Allow me to thank everyone involved in the work of IT4Innovations for their cooperation in 2016. At the same time, I would like to express my belief that in 2016 the next stage of positive development of IT4Innovations national supercomputing center has started. I hope that we maintain the goodwill of our users towards the IT4Innovations National Supercomputing Center, and that our supercomputers will continue to help them make breakthroughs in their research in the future.

Martin Palkovič
Managing director of IT4Innovations



IXPUG Workshop and Tutorials & Intel® PCC Meeting organized by IT4Innovations National Supercomputing Center 14-18 March 2016

IMPORTANT EVENTS IN 2016

In 2016 IT4Innovations participated in three international conferences as a local organizer. The **HiPEAC 2016** conference was organized in January in Prague and attracted more than 650 attendees. In March 2016 IT4Innovations organized the **IXPUG Workshop and Tutorials & Intel PCC Meeting** which was a week-long event held in Ostrava attended by over 60 participants from all over Europe and the USA. **PRACEdays16** and HPC Summit Week took place in Prague in May and were attended by over 200 participants.

Since mid 2016 we have been a member of the **European Technology Platform for High Performance Computing** (ETP4HPC), which focuses on the definition of research priorities for supercomputing. ETP4HPC issues and maintains a Strategic Research Agenda (SRA) to help the European Commission define the content of work programmes developing HPC technologies. Our membership in ETP4HPC enables us to influence the direction of Europe in the field of HPC and appropriately complements our membership in the pan-European research infrastructure Partnership for Advanced Computing in Europe (PRACE).

At the **Supercomputing 16** conference held annually in the United States, four IT4Innovations teams have succeeded with their research posters in worldwide competition. The ESPRESO team led by Lubomír Říha was among the five finalists aspiring to the best poster award.

Events for general public attracted nearly 1,300 visitors in 2016 and ranged from excursions of students, to the event called Researchers' Night, held in September all around Europe, for which IT4Innovations was host to over 500 visitors. Altogether there were 47 different events for the general public.

In the school year 2016/2017 we opened a new **Masters study programme Computational Sciences** and in September 2016 we welcomed our first students.

ORGANIZATION PROFILE

IT4Innovations National Supercomputing Center (IT4Innovations) is a research institute at VŠB – Technical University of Ostrava. We run state-of-the-art technology and provide supercomputer services to both Czech and foreign research teams from academia, research institutions and industry. We are also a research centre with strong international ties. The core topics of IT4Innovations' research are the processing and analysis of large data, the development of parallel scalable algorithms, engineering tasks, nanotechnology, and last but not least research focused on the development of infrastructure and supercomputer technologies. For the Czech scientific community, we provide a wide range of training sessions aimed at acquiring the knowledge needed to efficiently use our supercomputing infrastructure. We also think about the future, and within our Masters and Doctoral Study programmes, we educate new generations of supercomputing specialists to solve computationally challenging tasks in applied sciences and technologies.

Mission

Our mission is to deliver scientifically excellent and industry relevant research in the fields of high performance computing and embedded systems. We produce state-of-the-art technology and have expertise in high performance computing and embedded systems which we make available for Czech and international research teams from academia and industry.

Vision

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

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

Members:

- Dr. Ing. Martin Palkovič
- 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: Dr. Ing. Martin Palkovič

Members:

- Dr. Mgr. Branislav Janský
- Doc. Dr. Mgr. Vít Vondrák
- 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

IT4Innovations was created mainly thanks to European funding, specifically from the Operational Programme Research and Development for Innovation. The total subsidy provided was 1.47 billion CZK, 85 % of which was paid by the European Union and 15 % from the state budget of the Czech Republic. Between 2011 and 2015 the project 'Center of Excellence IT4Innovations' was jointly realized by five partners: VŠB – Technical University of Ostrava, The University of Ostrava, Silesian University in Opava, Brno University of Technology and the Institute of Geonics of the Czech Academy of Sciences. We continue to collaborate with these partners within the IT4Innovations Excellence in Science project, which is funded by the National Sustainability Programme II. Supervision of these two major projects is ensured by the Supervisory Board.

Supervisory Board

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

Vice-chairman: 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



Managing director
Martin Palkovič



Administration & Finances
Radim Mrázek



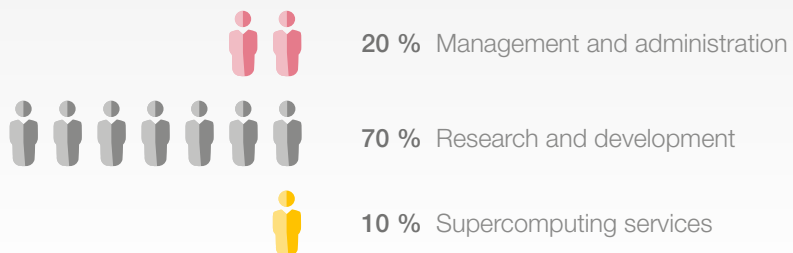
Research & Development
Vít Vondrák



Supercomputing Services
Branislav Janský

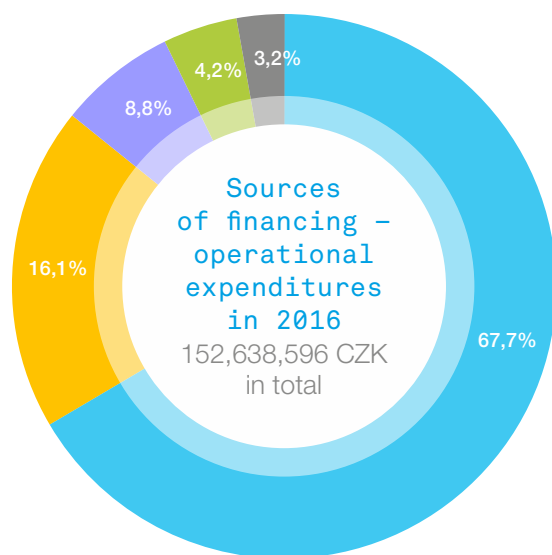
Employees of IT4Innovations

Employees of IT4Innovations by divisions in full time equivalent (FTE), 130 FTE in total



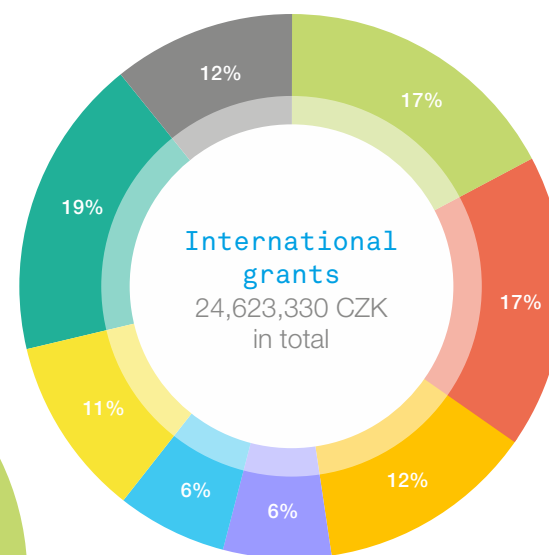
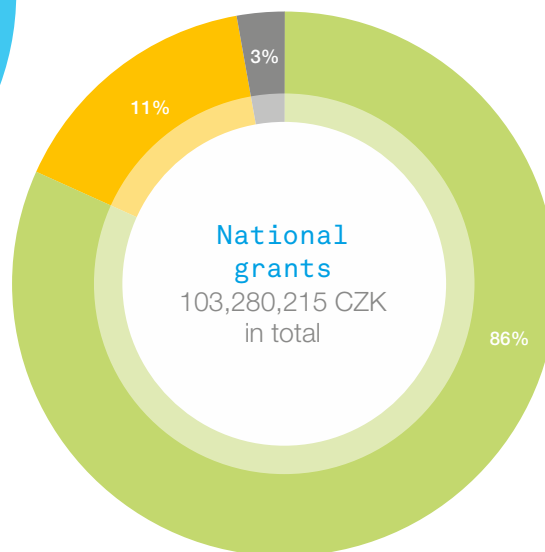
Sources of funding

In 2016 our overall budget was 154,806,506 CZK. 98.6 % of this amount was used for operational expenditures and 1.4 % was used for capital expenditures. National grants (targeted support) accounted for 67.7 % of the funding sources for operational expenditures. International grants accounted for 16.1 %, institutional support for 4.2 %, contract research together with renting computational resources for 3.2 % of the funding sources for operational expenditures. Other resources (8.8 %) include own sources, donations and income from contractual fines.



- National grants
- International grants
- Others
- Institutional support
- Contract research and renting computational resources

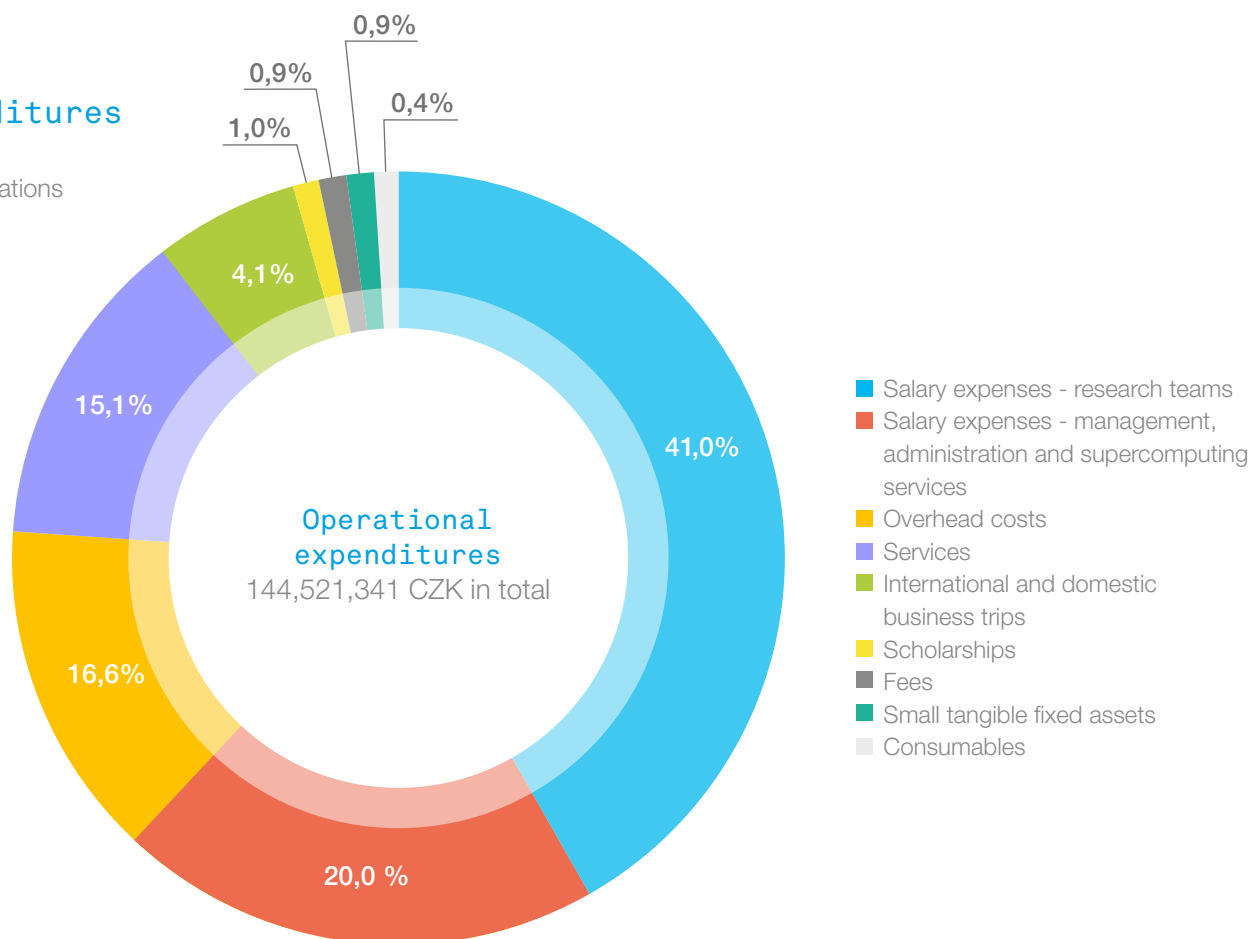
- Ministry of Education, Youth and Sports of the Czech Republic (15 projects)
- Technology Agency of the Czech Republic (4 projects)
- Grant Agency of the Czech Republic (2 projects)



- PRACE
- EXA2CT
- HARPA
- IPROCOT
- SESAME – NET
- READEX
- ExCAPE
- ANTAREX

Operational expenditures

Expenditures related to IT4Innovations operating activity amounted to 144,521,341 CZK. Salaries, overhead expenses and services amounted to almost 93 % of expenditures.



Summary of all grants

NATIONAL GRANTS

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

Large Infrastructures for Research, Experimental Development and Innovation project

- IT4Innovations National Supercomputing Center

National Sustainability Programme II project

- IT4Innovations Excellence in Science

Co-financing of the 7th Framework Programme of the European Union

- Harnessing Performance Variability
- EXascale Algorithms and Advanced Computational Techniques

Grants for specific university research

- Efficient implementation of boundary element method II
- Modeling of floods and pollution II
- Quantum methods in molecular physics
- Using HPC to analyze time series of uncertainties II
- Terahertz transitions in molecular crystals
- Enhancement of the tool for parallel segmentation of computer tomography and magnetic resonance imaging
- Using HPC for extensive computations in mechanics
- PERMON toolbox development II
- Use of HPC for transport optimization solutions with the involvement of dynamic routing II
- High parallel deep belief nets
- Vibration of the atomic lattice of actinide compounds

Projects supported by the Grant Agency of the Czech Republic

- New nonlinear and magneto-optical phenomena in periodic structures
- Effective methods of lifetime estimation for general multi-axis stresses

Projects supported by the Technology Agency of the Czech Republic

- Transport Systems Development Centre
- Integration of the SHM to system for ensurance of the continued airworthiness of a small transport aircraft
- Increasing Passengers Passive Safety and Comfort in Railway Traffic
- Center of competence for molecular diagnostics and personalized medicine

INTERNATIONAL GRANTS

Projects of the 7th Framework Programme for Research and Innovation of the European Union

- HARPA – Harnessing Performance Variability
- EXA2CT – Exascale Algorithms and Advanced Computational Techniques
- IPROCOT – The development of in silico process models for roll compaction

Projects of the 8th Framework Programme for Research and Innovation of the European Union - Horizon 2020

- ANTAREX – AutoTuning and Adaptivity appRoach for Energy efficient eXascale HPC systems
- READEX – Runtime Exploitation of Application Dynamism for Energy-efficient eXascale computing
- ExCAPE – Exascale Compound Activity Prediction Engine
- SESAME Net – Supercomputing Expertise for Small and Medium Enterprise Network
- PRACE 4IP – Partnership for Advanced Computing in Europe, 4th Implementation Phase

Others

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

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 currently operates two supercomputers - Anselm and Salomon.

Technical specifications of supercomputers

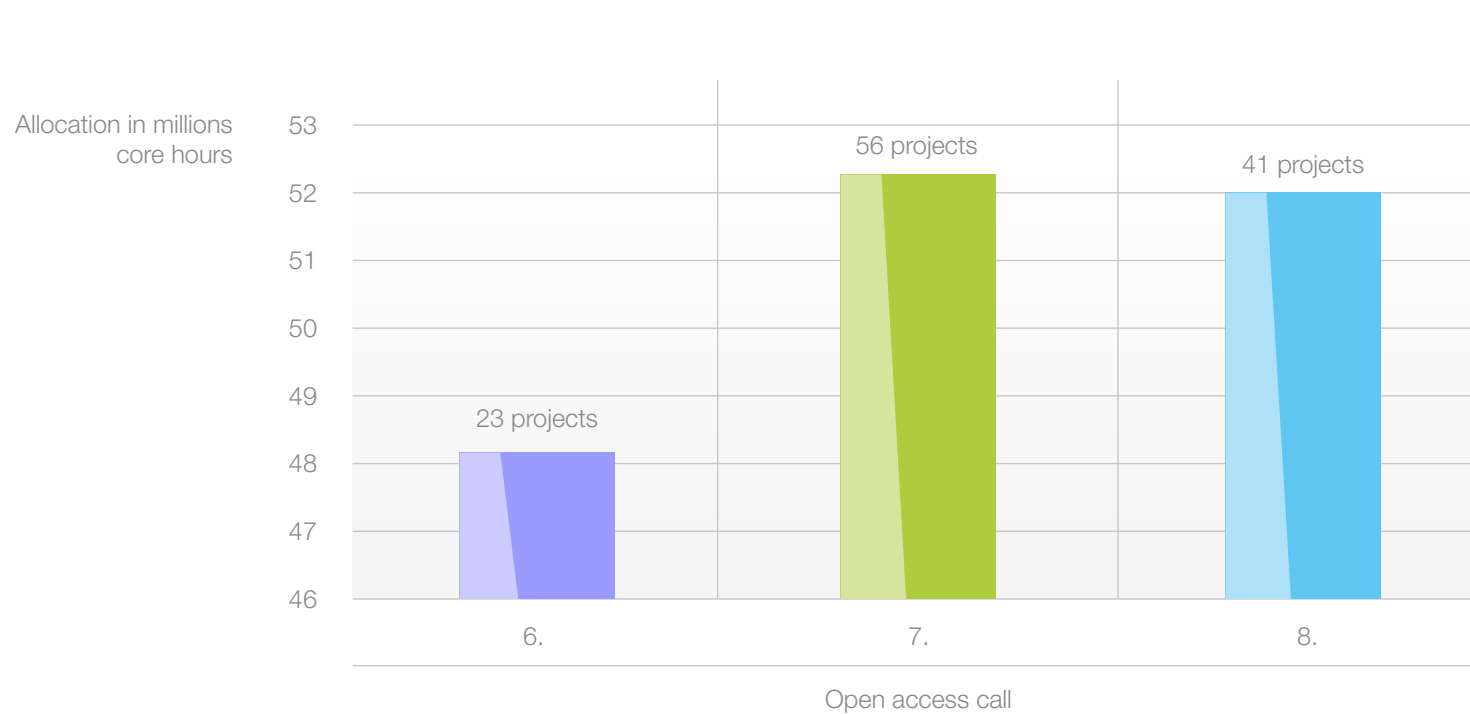
	ANSELM	SALOMON
Production	Spring 2013	Summer 2015, 67 th at TOP500 world supercomputers in November 2016
Peak performance	94 Tflop/s	2011 Tflop/s
Operating system	RedHat Linux 64bit 6.x	RedHat Linux 64bit 6.x, CentOS 64bit 6.x
Nodes	209	1008
CPU	2x Intel SandyBridge 8 cores 2.3/2.4 Ghz, 3344 cores in total	2x Intel Haswell 12 cores 2.5 Ghz, 24192 cores in total
RAM	64GB/96 GB/512 GB	128 GB/3.25 TB (UV node)
GPU accel.	23x NVIDIA Tesla Kepler K20	N/A
MIC accel.	4x Intel Xeon Phi 5110P	864x Intel Xeon Phi 7120P 61 cores each, 52704 cores in total
Storage	320 TiB /home (2 GB/s speed), 146 TiB /scratch (6 GB/s speed)	500 TiB /home (6 GB/s speed), 1638 TiB /scratch (30 GB/s speed)
Interconnection	Infiniband QDR 40 Gb/s	Infiniband FDR 56 Gb/s

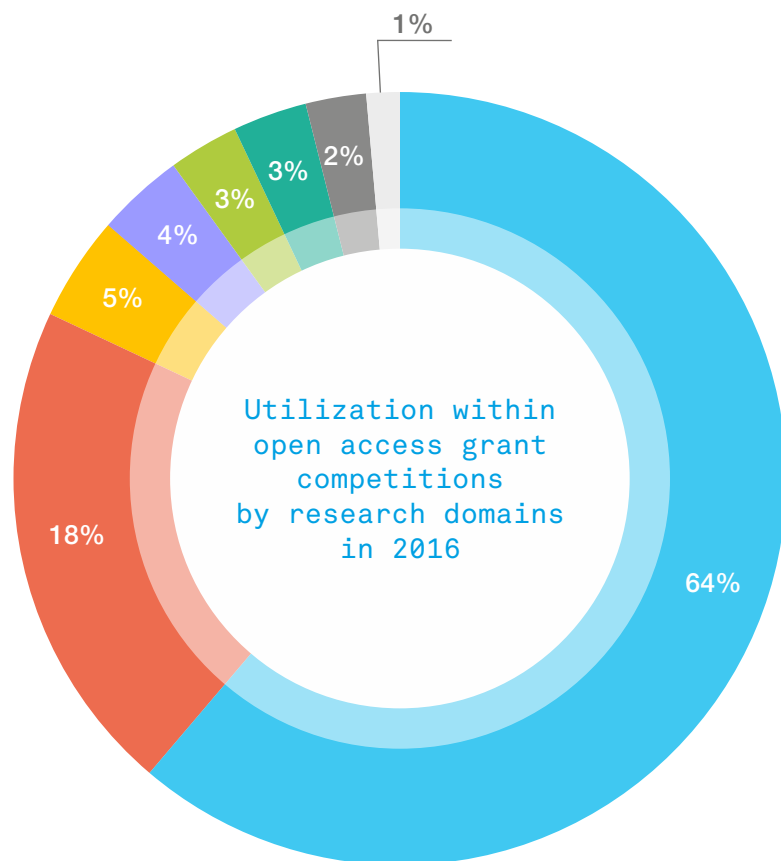
Computational resources allocation

Computational resources of IT4Innovations are dedicated for solving tasks from research and development done by academic and research institutions. Part of the capacity is also devoted to the development of cooperation between academia and industry, and to independent use by industrial enterprises.

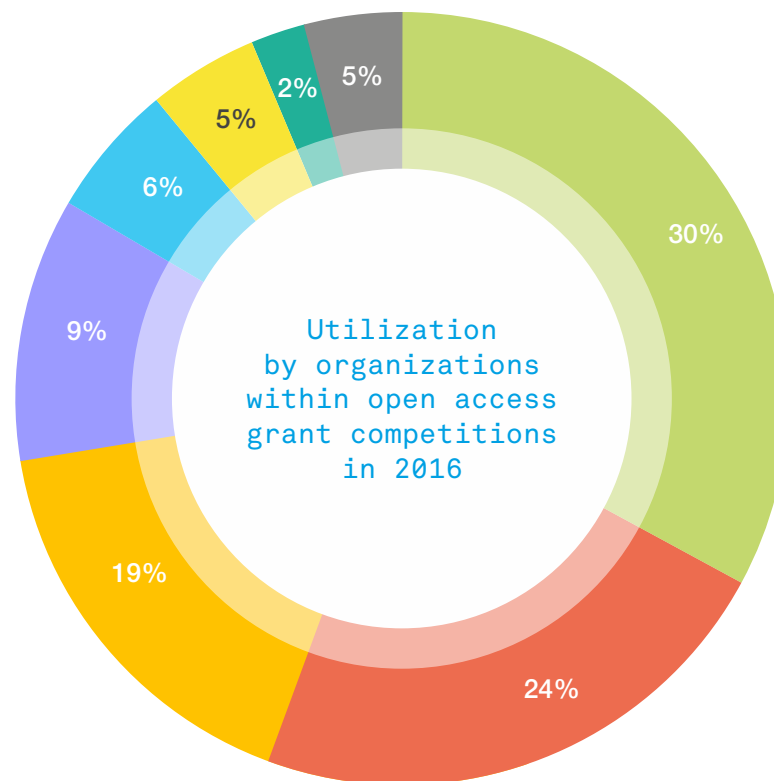
Institutions can apply for computation time within open access grant competitions. Open access competitions are announced three times a year. In 2016, within the open access competitions we allocated 152,388,700 core hours among 120 research projects enhancing Czech science. Core hours demand exceeded the supply by 14.2 %.

Open access grant competitions in 2016





Material Sciences	Informatics
Bio Sciences	Astrophysics
Physics	Engineering
Applied Mathematics	Earth Sciences



IT4Innovations	Brno University of Technology
Research Institutes of The Czech Academy of Sciences (7)	Czech Technical University in Prague
CEITEC	Masaryk University
Charles University	Others (10)

Computation time can be also granted upon request, at discretion of directors. An application can be made at any time, and computing time is assigned irregularly based on an IT4Innovations management assessment. Representatives from both commercial and non-commercial spheres can apply in cases when open access grant competitions cannot be used. Based on a decision by the management, a total of 3,170,834 core hours were allocated to 21 projects in 2016.

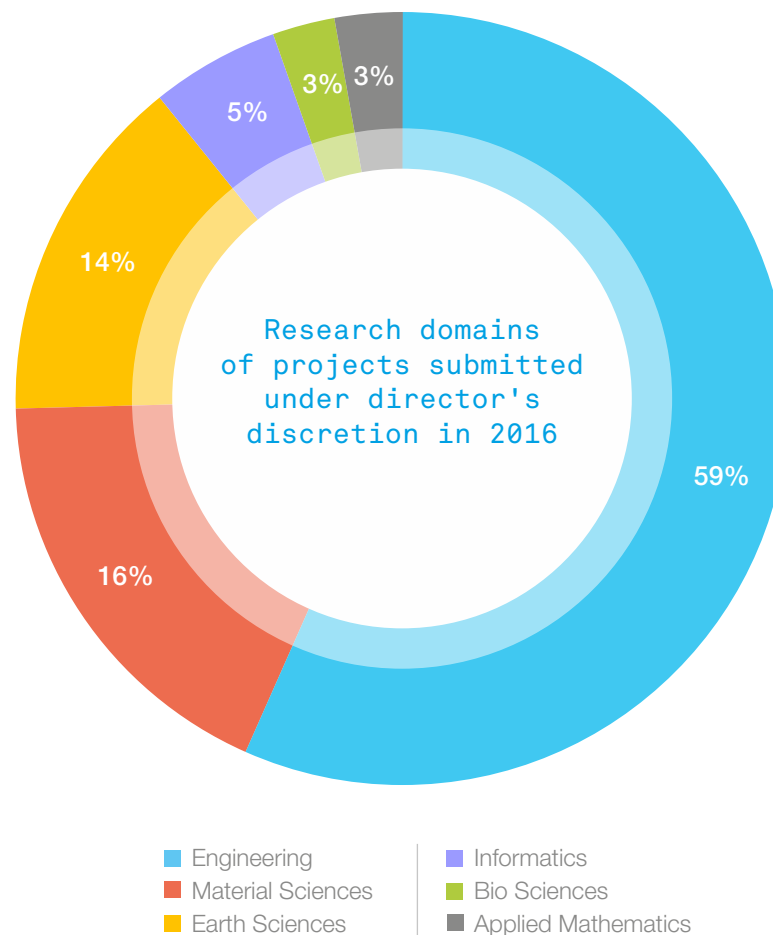
Institutions can also rent the computational resources. In 2016, two companies rented the computation time of our clusters, for almost 3,000,000 CZK.

Users of computational resources

The number of active users was 310 in total in 2016.

Our technical support received 1126 queries in 2016. 1121 were successfully resolved. Five were rejected.

Internal response time (24h for first response) was observed at 98.4% of requests. The internal closure time, which may not be longer than 30 days, was observed for 95.3% of requests.



Projects

Several national and international grants helped 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. An important international project in which we are involved is PRACE (Partnership for Advanced Computing in Europe), which was already in implementation phase 4 in 2016.

NATIONAL GRANTS

IT4Innovations National Supercomputing Center (2016 – 2019)

Project ID: LM2015070

Principal investigator: Dr. Ing. Martin Palkovič

The aim of the project is to operate the most powerful and state-of-the-art supercomputer systems in the Czech Republic and to provide open access to these resources based on research excellence. Supercomputing and High Performance Computing (HPC) are the third key science pillar in addition to theoretical and experimental research. In recent years, supercomputers have become increasingly important and are often the only option, especially when the experiment is not possible. Computer simulations are often cheaper, faster and safer or more environmentally friendly than the experiment. The IT4Innovations portfolio is divided into so-called basic services and so-called value-added services. Basic services consist of providing an optimized supercomputing environment, namely supercomputer core hours, software licenses, and data repositories needed to implement the calculations. Value-added services are based on IT4Innovations

expertise, including user and application support, parallel code development and optimization, training activities, own research of the infrastructure, and providing a contact point for international HPC infrastructures. As part of the PRACE (Partner for Advanced Computing in Europe) e-Infrastructure IT4Innovations provides Czech researchers with access to all services and expertise of this e-Infrastructure and opens opportunities for international cooperation.

<http://www.msmt.cz/vyzkum-a-vyvoj-2/cestovni-mapa-cr-velkych-infrastruktur-pro-vyzkum>

INTERNATIONAL GRANTS

PRACE-4IP – Partnership for Advanced Computing in Europe,
4th Implementation Phase (2015 - 2017)

Project ID: 653838 (H2020-EINFRA-2014-2 call)

Co-investigator: Doc. Dr. Mgr. Vít Vondrák

The aim of the project is to build on the success of previous PRACE projects by continuing to develop cooperation across the field of supercomputing, to strengthen the competitiveness of European science, research, and industry.

<http://www.prace-ri.eu/prace-4ip/>

SESAME - NET – Supercomputing Expertise for Small and Medium
Enterprise Network (2015 – 2017)

Project ID: 654416 (H2020-EINFRA-2014-2 call)

Co-investigator: Dr. Ing. Tomáš Karásek

The aim of this project is to establish a network of centres mutually cooperating and supporting small and medium-sized enterprises in exploitation of HPC for their development. Within the scope of this project, educational materials, manuals, and an educational events portfolio, which will be freely available in all European countries, will be prepared.

<https://sesamenet.eu/>

CzeBaCCa – Czech-Bavarian Competence Team for
Supercomputing Applications

Co-investigators: Dr. Ing. Martin Palkovič, Doc. Dr. Mgr. Vít Vondrák,
Dr. Mgr. Branislav Janský

CzeBaCCA is the Czech-Bavarian Competence Team for Supercomputing Applications. With the next generation of supercomputers coming up by the early 2020s, it is imperative to optimise simulation codes and at the same time to start training domain scientists. Only that way will it be possible to best exploit the upcoming high performance systems capable of 10^{18} FLOPS. In 2016 CzeBaCCA organized the following seminars that helped to exchange experience and knowledge:

in Ostrava:

- Intel MIC Programming Workshop
- Scientific Workshop: SeisMIC - Seismic Simulation on Current and Future Supercomputers

in Garching:

- PRACE PATC Course: Intel MIC Programming Workshop
- Scientific Workshop: High Performance Computing for Water Related Hazards

<https://www.lrz.de/forschung/projekte/forschung-hpc/CzeBaCCA/>



RESEARCH & DEVELOPMENT

RESEARCH & DEVELOPMENT

At the end of 2015, the project 'Center of Excellence IT4Innovations', supported by the Operational Programme Research and Development for Innovations, was concluded. This project has funded the establishing of the center, the acquisition of infrastructure and the operation of the Center since 2011. The project defined eight research programmes, each with a different focus. Certain research programmes have been organizationally transferred to partner institutions involved in the original project, or merged. That is why we started the process of restructuring the research programmes within the IT4Innovations research institute at VŠB – Technical University of Ostrava in 2016. As of 1 January 2017, we have renamed our research programmes so that the names correspond with the new focus and each team's research activities. Teams are not called research programmes anymore, but we are using laboratories instead. Since January 2017, we have also set up the Laboratory for Infrastructure Research, to strengthen and focus our own infrastructure research.

Research programme	Laboratory	Abbreviation	Head of laboratory
HPC Libraries and Supercomputing for Industry	Parallel Algorithms Research Lab	PAR	Prof. T. Kozubek
IT for Disaster and Traffic Management	Advanced Data Analysis and Simulations Lab	ADAS	Dr. J. Martinovič
Modelling for Nanotechnologies	Modelling for Nanotechnologies Lab	NANO	Prof. J. Pištora
IT for Knowledge Management	Big Data Analysis Lab	BIGDATA	Prof. V. Snášel
	Infrastructure Research Lab (new since 2017)	INFRA	Dr. B. Jansík

Laboratories and their staff (in FTE)

Research programme / Lab	PAR	ADAS	NANO	BIGDATA
Head of research lab	1	1	0,5	0,5
Senior researcher	5	3,22	1	0
Researcher	14,41	10,08	2,1	2,26
Research Assistant	13,59	10,23	3,19	2,31
External Specialist	2,2	0,5	1,68	2,03
R&D Support Staff	4,59	5,53	0	4,43
Total	40,79	30,56	8,47	11,53



Parallel Algorithms Research Lab

Research programme HPC Libraries and Supercomputing for Industry

The principal objective of the laboratory is to develop in-house libraries of efficient parallel algorithms based on advanced computational techniques and HPC technologies (ESPRESO, BEM4I, MULTIDYN, MCSIMUL, and PIMCSIMUL). These libraries are used to solve extremely difficult problems in engineering and molecular dynamics and to support the respective communities.

The second principal objective is the collaboration and support of industrial partners. This goal is fulfilled through contract research, joint research projects, and capability development. The above in-house libraries and selected commercial and open source third party software packages are applied to solve the problems challenging our partners. Cooperation and HPC services are offered to users from the application area using our web portal <http://industry.it4i.cz/en>.

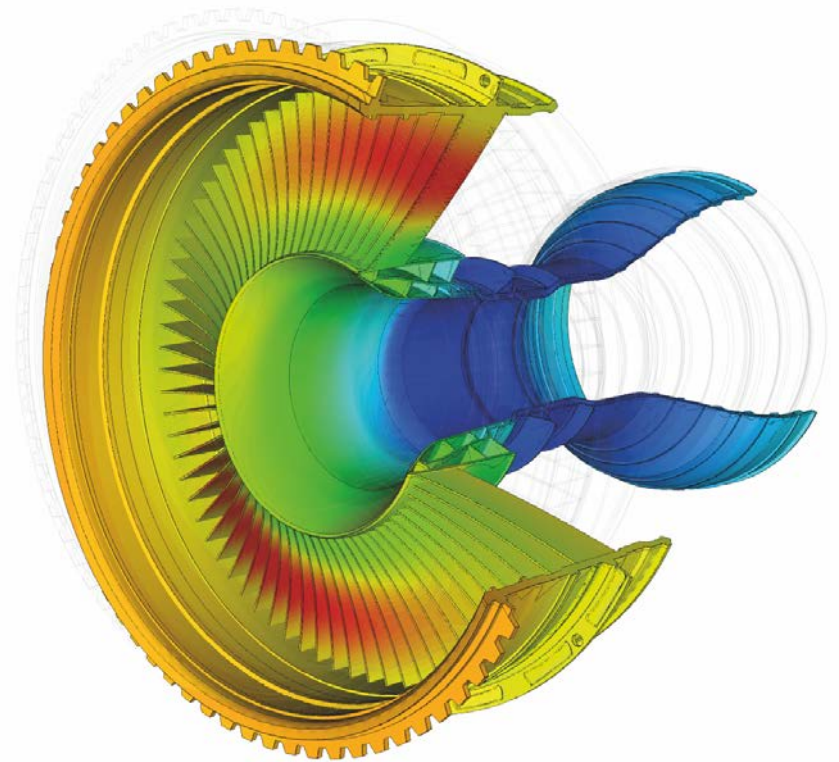
Significant events in 2016

- Petr Horyl, Tomáš Karásek, Petr Ferfecki a Pavel Maršálek won the HiPEAC Technology Transfer Award for the technology transfer project called "Improved passive safety and comfort of passengers in railway traffic" on which they cooperated with the company BORCAD.

Selected publications in 2016

- Zapoměl, J., Stachiv, I., Ferfecki, P.: A novel method combining Monte Carlo-FEM simulations and experiments for simultaneous evaluation of the ultrathin film mass density and Young's modulus, (2016) Mechanical Systems and Signal Processing, 66-67, pp. 223-231.
DOI: 10.1016/j.ymssp.2015.06.022, IF 2.771, Q1.
- Halama, R., Fusek, M., Poruba, Z.: Influence of Mean Stress and Stress Amplitude on Uniaxial and Biaxial Ratcheting of ST52 Steel and Its Prediction by the AbdelKarim–Ohno Model. International Journal of Fatigue 91 (2), 2016, pp. 313-321.
DOI: 10.1016/j.ijfatigue.2016.04.033, IF 2.1, Q1.

- Benhenni, M., Stachoř, M., Gadéa, F. X., Yousfi, M., Kalus, R.: Transport and dissociation of neon dimer cations in neon gas: a joint dynamical and Monte Carlo modeling, (2016) Journal of Physics B: Atomic, Molecular, and Optical Physics, vol. 49, Art. No. 175205.
DOI: 10.1088/0953-4075/49/17/175205, IF 1.833, Q2.
- Říha, L., Brzobohatý, T., Markopoulos, A., Jarošová, M., Kozubek, T., Horák, D., Hapla, V.: Implementation of the efficient communication layer for the highly parallel total FETI and hybrid total FETI solvers, (2016) SIAM Parallel Computing, 57, pp. 154-166.
DOI: 10.1016/j.parco.2016.05.002, IF 1,0, Q3.
- Dostál, Z., Kozubek, T., Sadowská, M., Vondrák, V.: Scalable Algorithms for Contact Problems, DOI: 10.1007/978-1- 4939-6834-3, book in Springer-Verlag New York.



Structural integrity of aircraft engine parts



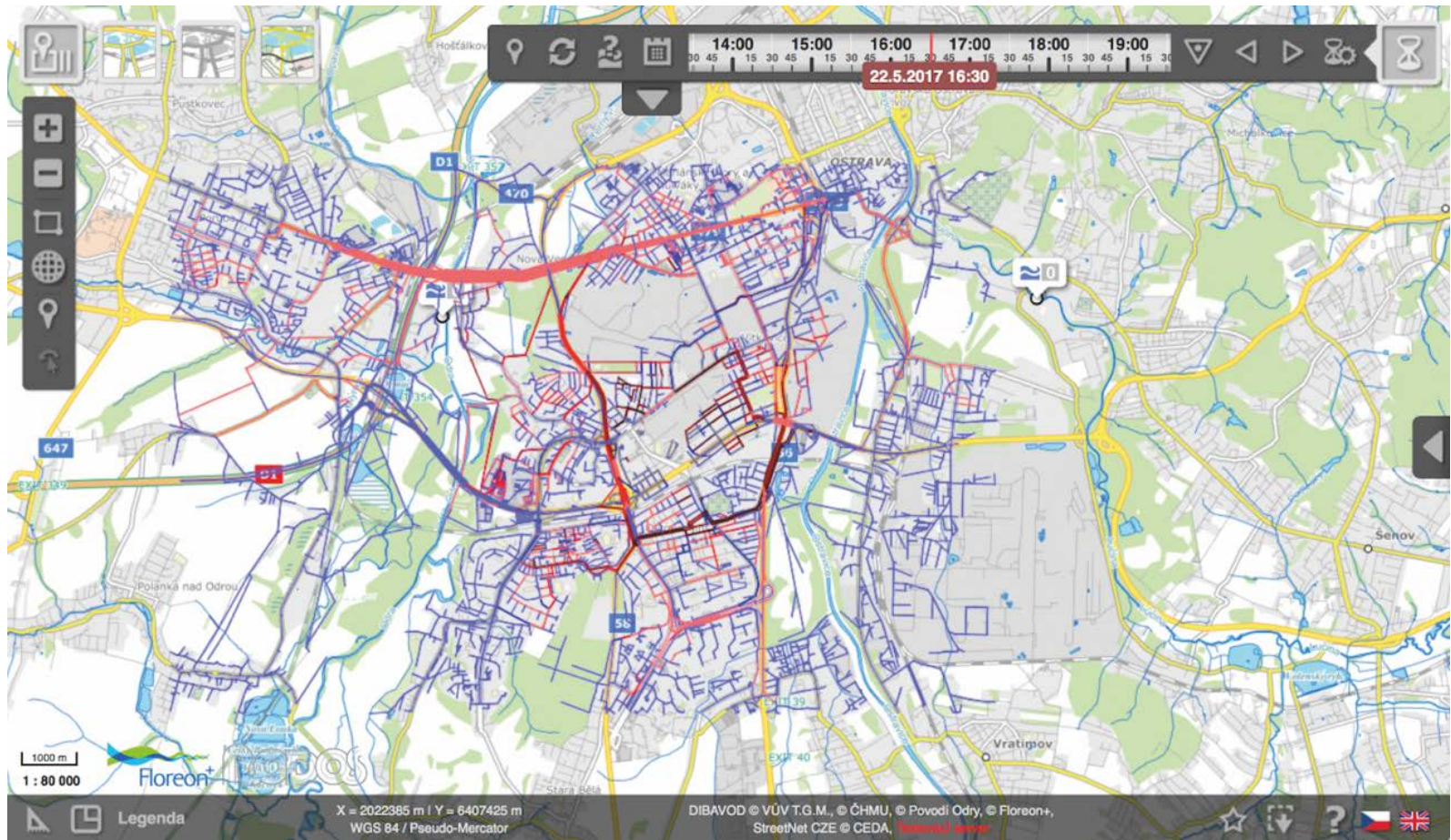
Advanced Data Analysis and Simulations Lab

Research programme IT for Disaster and Traffic Management

The main objective of this laboratory is to design and implement an HPC platform for decision making in crisis management and industry. This platform will be provided as a service to internal and external users, will utilize the computing power of HPC infrastructures, collect, store, and pre-process data into specialized data structures, and provide user-understandable visualization of results. Another important objective is the research and development of scalable models to simulate the behaviour of dynamic systems. An example of such systems is modelling in crisis or traffic management. Simulations of such systems are often based on incomplete or inaccurate data, heuristics, and therefore the developed models will take into account the probabilistic aspects of input parameters. Inverse methods will be used for optimal setting of unknown input parameters along with statistical analysis of historical data. Communication interfaces will also be developed to integrate custom computational models into the platform.

Selected publications in 2016

- Lampart, M., Oprocha, P.: Chaotic sub-dynamics in coupled logistic maps, (2016) *Physica D: Nonlinear Phenomena*, 335, pp. 45-53. DOI: 10.1016/j.physd.2016.06.010. IF 1,579, Q1
- Martinovic, T.: Chaotic behaviour of noisy traffic data, (2016) *Mathematical Methods in the Applied Sciences*, DOI: 10.1002/mma.4234. IF 1,002, Q2
- Reznar, T., Martinovic, J., Slaninova, K., Grakova, E., Vondrak, V.: Probabilistic Time-Dependent Vehicle Routing Problem, (2016) *Central European Journal of Operations Research*. DOI: 10.1007/s10100-016-0459-2. IF 0,978, Q3
- Martinovic, J., Slaninova, K., Golasowski, M., Cmar, R., Cardoso, J. M. P., Bispo, J., Palermo, G., Gadioli, D., Silvano, C.: DSL and Autotuning Tools for Code Optimization on HPC Inspired by Navigation Use Case, (2016), Poster, SC16: International Conference for High Performance Computing, Networking, Storage and Analysis, November, Salt Lake City, UT, USA
- Böhm, S., Meca, O., Jančar, P.: State-space reduction of non-deterministically synchronizing systems applicable to deadlock detection in MPI, (2016) *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, 9995 LNCS, pp. 102-118. DOI: 10.1007/978-3-319-48989-6_7



Traffic modelling with the Floreon+ system



Modelling for Nanotechnologies Lab

Research programme Modelling for Nanotechnologies

The activities of the Modelling for Nanotechnologies laboratory are oriented towards HPC applications that support experimental aspects of nanotechnologies. Laboratory research is focused on new materials and is conceived by a compact unit consisting of physical and chemical laboratories. They provide research in the field of nanotechnologies, proprietary technology bases for the preparation of nanostructures, measuring and diagnostic assemblies, and application blocks.

Research areas include new terahertz sources, plasmonics and non-reciprocal photon structures, photovoltaics and security diffraction structures, spin lasers, optical and magneto-optical phenomena in periodic structures and nanostructures, anharmonic grating vibration effects, low-dimensional materials and interfaces of materials, magneto-optically active materials and structures, and design of nuclear fuels for IV generation reactors.

Significant events in 2016

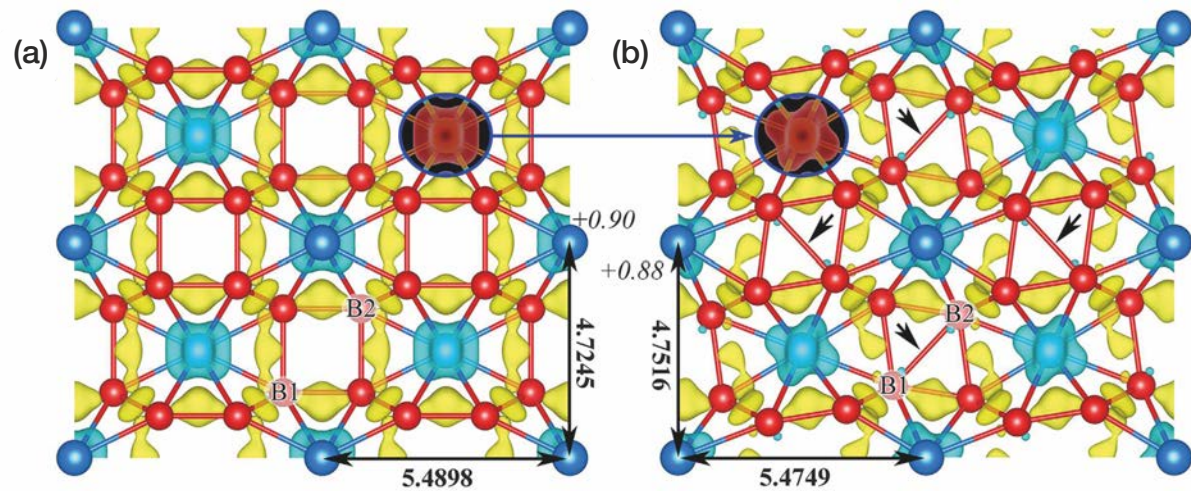
- Ing. Šárka Kunčická won third place in the Werner von Siemens competition for her diploma thesis "Deposition and characterization of Y-substituted BiG thin films"
- Publication: N. Nguyen-Huu, J. Pištora, M. Cada: Wavelength-selective emitters with pyramid nanogratings enhanced by multiple resonance modes. Nanotechnology 27, 155402, DOI: 10.1088 / 0957-4484 / 27/15/155402 (2016) was awarded as "Featured article"

Selected publications in 2016

- N. Nguyen-Huu, J. Pištora, M. Cada: Wavelength-selective emitters with pyramid nanogratings enhanced by multiple resonance modes. Nanotechnology 27, 155402, DOI: 10.1088/0957-4484/27/15/155402 (2016), IF 3.573, Q1
- R. F. Zhang, X. D. Wen, D. Legut, Z. H. Fu, S. Veprek, E. Zurek, H. K. Mao: Crystal Field Splitting is Limiting the Stability and Strength of Ultraincompressible Orthorhombic Transition Metal Tetraborides, Scientific Reports 6, 23088; DOI: 10.1038/srep23088 (2016), IF 5.228, Q1
- O. Stejskal, J. Hamrle, J. Pištora, Y. Otani: Optimization of spin injection and spin detection in lateral nanostructures by geometrical means, Journal of Magnetism and Magnetic Materials 414 (2016) 132–143, DOI: 10.1016/j.jmmm.2016.04.051, IF 2.357, Q2

- Z. J. He, Z. H. Fu, D. Legut, X. H. Yu, Q. F. Zhang, V. I. Ivashchenko, S. Veprek, R. F. Zhang: Tuning lattice stability and mechanical strength of ultraincompressible tungsten carbides by varying the stacking sequence, PHYSICAL REVIEW B 93, 184104 (2016), DOI: 10.1103/PhysRevB.93.184104, IF 3.719, Q1
- K. M. Lebecki, D. Legut: Fast vortex core switching at high temperatures, Journal of Magnetism and Magnetic Materials 411 (2016) 7–11, DOI: 10.1016/j.jmmm.2016.03.025, IF 2.357, Q2

Picture from the scientific article
 „Crystal Field Splitting is Limiting
 the Stability and Strength
 of Ultraincompressible Orthorhombic
 Transition Metal Tetraborides“
 in Scientific Reports 6, 23088;
 DOI: 10.1038/srep23088 (2016).





Big Data Analysis Lab

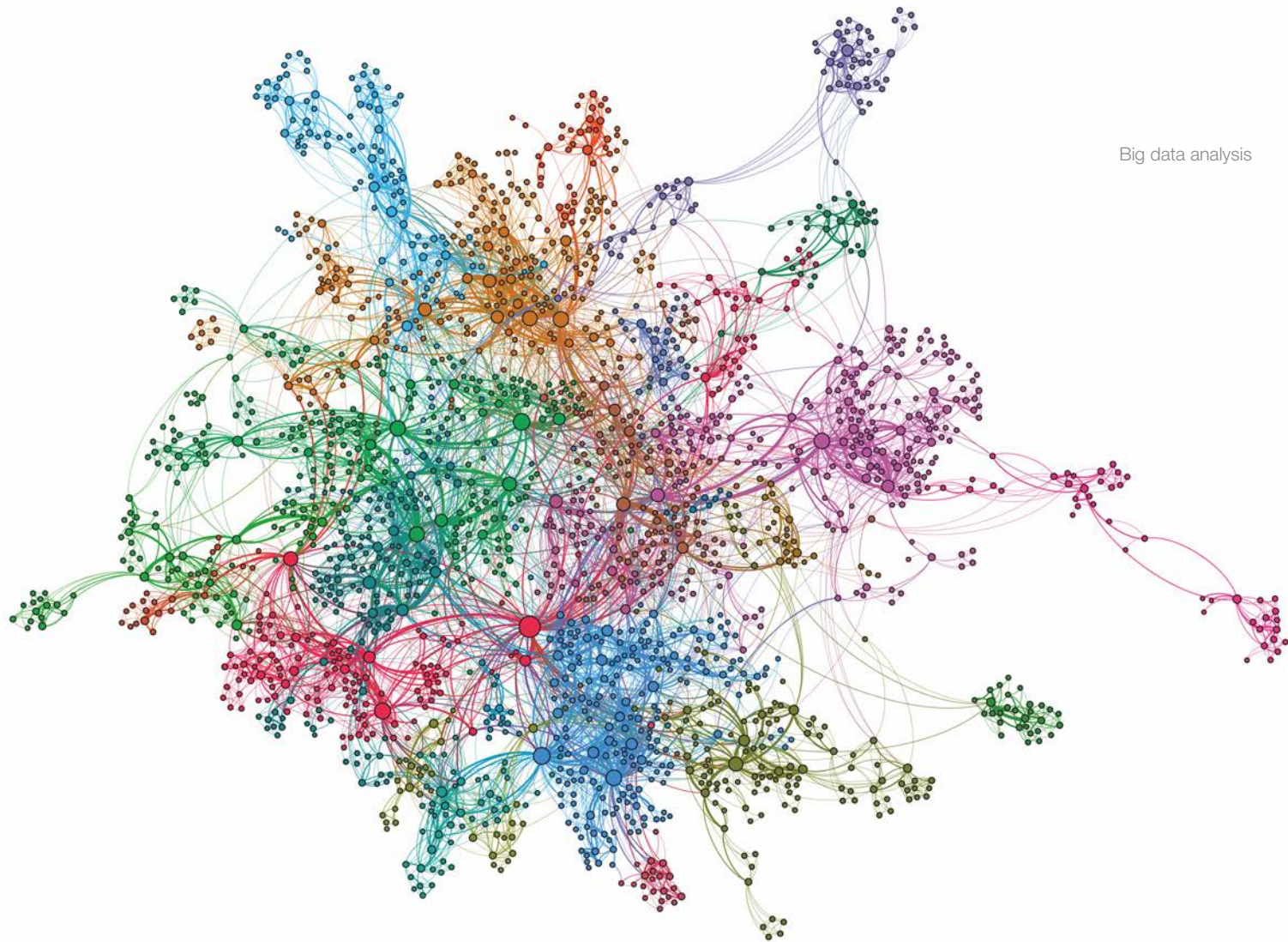
Research programme IT for Knowledge Management

There are two major research areas of the laboratory. The activities concerned with big data analysis are focused on the development of novel knowledge extraction tools suitable for very large collections of challenging (noisy, weakly-structured) data and data sources with large speed of content generation (data streams). The investigated approaches are built mainly on formal topological and statistical methods that require careful parallelization in order to scale for big data.

The second research area deals with mobile device security and safety. Although the research is centred around the situation in the Czech Republic, the obtained results can be used worldwide due to the universality of the topic. Modern mobile devices often combine information about location with sensitive personal data. This type of data obtained advanced security and vulnerability screenings and analyses. Achieving a secure mobile ecosystem is a multi-layer objective that requires orchestration of network-level, operator-level, device-level, and application-level security. Security analyses that consider all these aspects and can contribute to mitigation of at least the major threats were part of the research programme focus for the year 2016.

Selected publications in 2016

- Zjavka, L., Pedrycz, W.: Constructing General Partial Differential Equations using Polynomial and Neural Networks. (2016) Neural Networks. Vol. 73, p.58–69. DOI: 10.1016/j.neunet.2015.10.001. IF 3.216, Q1
- Zjavka, L., Snášel, V.: Short-term power load forecasting with ordinary differential equation substitutions of polynomial networks. (2016) Electric Power Systems Research. Vol. 137, p. 113–123. DOI: 10.1016/j.epsr.2016.04.003. IF 1.809, Q2



Big data analysis

Projects

NATIONAL GRANTS

IT4Innovations Excellence in Science (2016 - 2020)

Project ID: LQ1602

Principal investigator: Dr. Ing. Martin Palkovič

The main objective of the project is to build on the research activities successfully launched within the framework of the Operational Programme Research and Development for Innovations Center of Excellence IT4Innovations and further increase the scientific excellence and international impact of these research activities, especially in the areas of "High Performance Computing" (HPC) and "Cyber-physical systems", and related sciences such as computational sciences, mathematics, biomedicine, engineering, material sciences, or Earth sciences. An integral part of this goal is the extensive use of the supercomputing infrastructure that makes the center a leading European HPC center and development of applications for its efficient use. This infrastructure is also recognized as the Czech National e-Infrastructure - IT4Innovations National Supercomputing Center - on the Czech Republic's Road Map of Large Infrastructures for Research, Experimental Development and Innovation. The research team thus gains access to a high-quality research infrastructure, the potential of which will be used both to improve the quality of its own R & D results and to establish cooperation with other important national and international institutions and in particular with the application sphere. Further personnel development of the center will be supported by educational and dissemination activities in the research domain of the Center.

GRANTS FOR SPECIFIC UNIVERSITY RESEARCH

Efficient implementation of boundary element method II (2016)

Project ID: SP2016/113

Principal investigator: Dr. Ing. Michal Merta

The aim of the project was to further develop the existing library of parallel solvers based on the Boundary Element Method BEM4I.

Modelling of floods and pollution II (2016)

Project ID: SP2016/150

Principal investigator: Dr. Ing. Tomáš Brzobohatý

The project extends previous specific research on Flood and Pollution Modelling. The research team continued with connecting several scientific disciplines, which are linked to numerical solutions of risk-prediction tasks such as leaks and dispersion of hazardous substances.

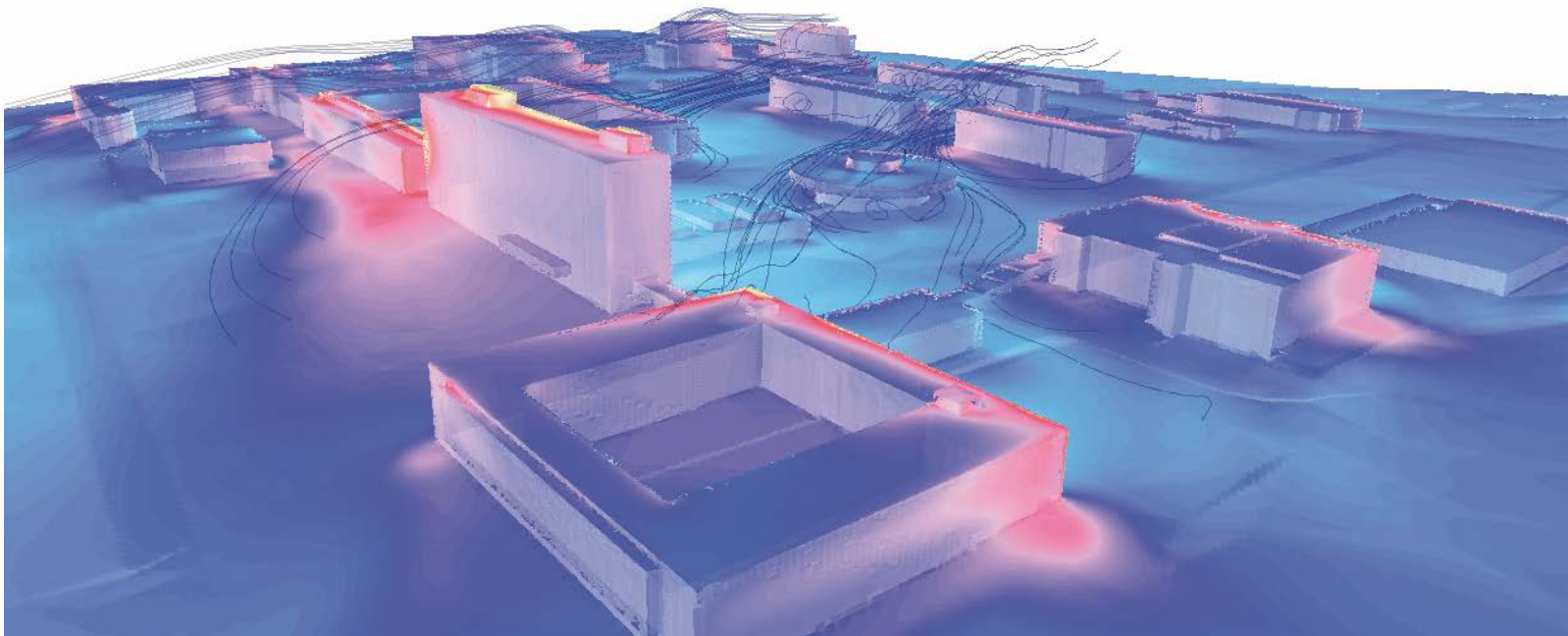
Quantum methods in molecular physics (2016)

Project ID: SP2016/157

Principal investigator: Doc. Dr. RNDr. René Kalus

The project was focused on the use of mathematical methods and supercomputing methods in molecular physics with the main emphasis on modeling of quantum effects in small atomic clusters.

Flow simulation over VŠB - Technical University of Ostrava campus



Using HPC to analyze time series of uncertainties II (2016)

Project ID: SP2016/166

Principal investigator: Dr. Ing. Kateřina Slaninová

The aim of the project was the implementation of algorithms to enable efficient prediction and comparison of indefinite time series with the emphasis on the use of parallelization to accelerate the computations.

Terahertz transitions in molecular crystals (2016)

Project ID: SP2016/167

Principal investigator: Doc. Dr. Mgr. Kamil Postava

Within the project the molecular crystalline spectroscopy in powder and crystalline form in the terahertz and infrared areas was studied. The study was focused on changes in the populations of vibrational states of hydrogen bonds in the terahertz region when they were excited using an infrared laser.

Enhancement of the tool for parallel segmentation of computer tomography and magnetic resonance imaging (2016)

Project ID: SP2016/171

Principal investigator: Dr. Ing. Tomáš Karásek

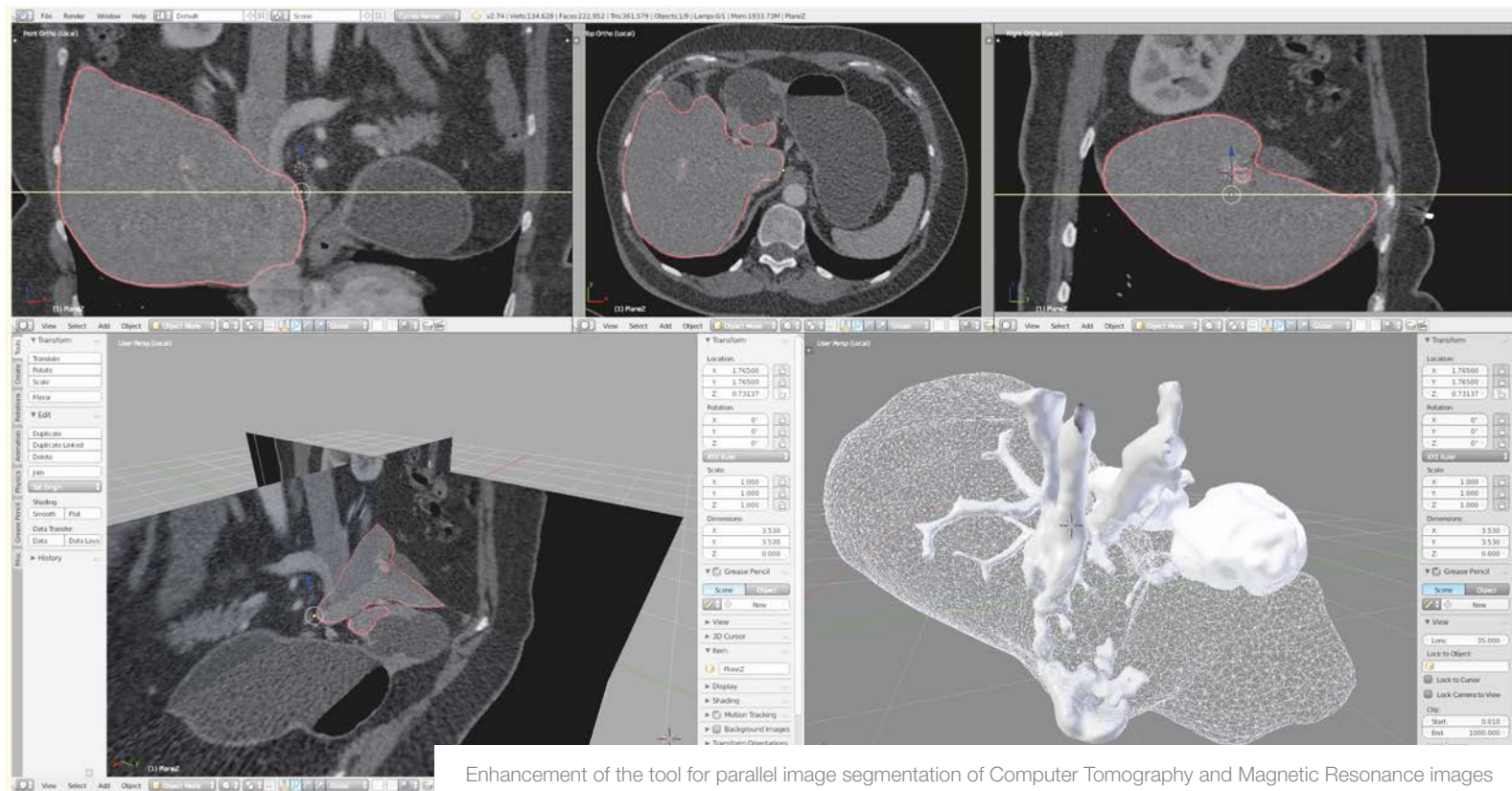
The aim of this project was to implement algorithms for digital image processing with a focus on human organ recognition from computer tomography and magnetic resonance imaging.

Using HPC for extensive computations in mechanics (2016)

Project ID: SP2015/113

Principal investigator: Prof. Dr. Ing. Petr Horyl, dr.h.c.

The project focused on strength optimization of wheelchairs for immobile patients, modelling the interaction of a sitting and lying patient with the wheelchair construction, and crash test modeling for aircraft seats.



PERMON toolbox development II (2016)

Project ID: SP2016/178

Principal investigator: Doc. Dr. Ing. David Horák

Within the project the PERMON tool set was further developed. PERMON uses the latest theoretical knowledge in the field of discretization techniques, quadratic programming algorithms and domain decomposition methods.

Use of HPC for transport optimization solutions with the involvement of dynamic routing II (2016)

Project ID: SP2016/179

Principal investigator: Dr. Ing. Jan Martinovič

The project dealt with the transport optimization and the dynamic planning of vehicle routes by using HPC. Routing algorithms were improved, as well as solutions related to the processing and storage of necessary data.

High Parallel Deep Belief Nets (2016)

Project ID: SP2016/180

Principal investigator: Ing. Petr Buček

Within the project high-parallel methods were developed, as deep belief nets are able to take into account millions of parameters for recognizing complex shapes under permanent resistance to learning.

Vibration of the atomic lattice of actinide compounds (2016)

Project ID: SP2016/182

Principal investigator: Dr. Ing. Dominik Legut

The project included study of thermodynamic stability of defect-free and defective compounds due to radiation effects, temperature behavior prediction, spin-orbital interaction effect, and Coulomb interaction size on lattice vibration states.

PROJECTS SUPPORTED BY THE GRANT AGENCY OF THE CZECH REPUBLIC

New nonlinear and magneto-optical phenomena in periodic structures (2016 – 2017)

Project ID: GA15-08971S

Co-investigator: Doc. Dr. Mgr. Kamil Postava

Within the project the generation of quantum-correlated photon pairs in modern photonic structures is studied, especially in non-linear thin-film metal-dielectric structures, in magneto-optical periodic structures and periodically-polar structures.

Effective methods of lifetime estimation for general multi-axis stresses (2015 – 2017)

Project ID: GA15-18274S

Principal investigator: Doc. Dr. Ing. David Horák

The project focuses on methods for predicting fatigue life for multi-axis loading in the field of low cycle fatigue, i.e. in cases where plasticity can not 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 will be converted into a fully parallel scalable application.

PROJECTS SUPPORTED BY THE TECHNOLOGY AGENCY OF THE CZECH REPUBLIC

Transport Systems Development Centre (2012 – 2018)

Project ID: TE01020155

(project of the Competence centre programme)

Principal investigator: Prof. Dr. Ing. Ivo Vondrák

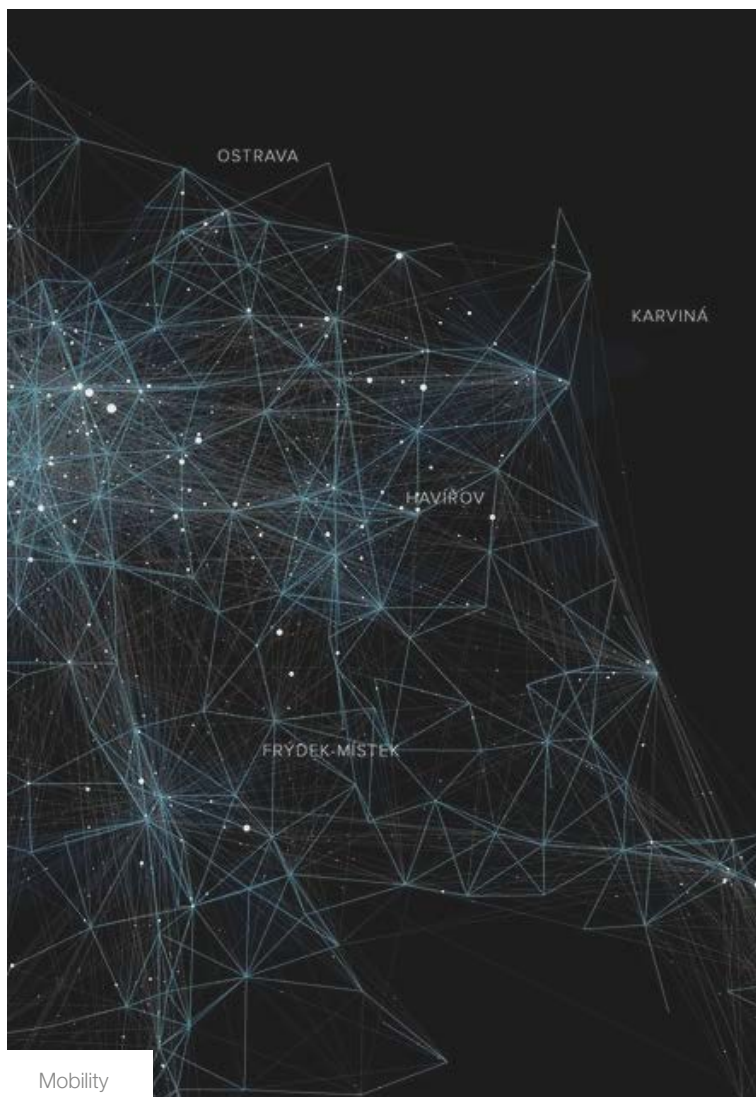
The Transport Systems Development Centre creates a strategic partnership of cooperating research institutions and businesses that determine the development direction of smart mobility in the Czech Republic. Together, we have embraced the challenge of finding a balance between the importance of transportation in modern society and the negative impact of mobility. We rely on experienced teams, perfect knowledge of the environment, willingness to cooperate and share the risks associated with adjusting the mobility management trends to 21st century needs.

Integration of the SHM to system for ensurance of the continued airworthiness of small transport aircraft (2013 – 2016)

Project ID: TA03010140 (Alfa programme project)

Co-investigator: Doc. Dr. Ing. Dalibor Lukáš

The project focused on the system development for automatic real-time aeroplane monitoring, based on the analysis of surface ultrasound wave distribution in the primary elements of the structure and its integration into the continuing airworthiness system of a small aeroplane.



Mobility

Increasing Passengers Passive Safety and Comfort in Railway Traffic (2014 – 2017)

Project ID: TA04031236 (Alfa programme project)

Principal investigator: Prof. Dr. Ing. Petr Horyl, dr.h.c.

The aim of the project was to design and produce functional double seats for long-distance and regional rail passenger's transport. The double seat met the revised parameters of British crash - test standards GM/RT2100 and was addressed in the first phase for the UK market.

Center of competence for molecular diagnostics and personalized medicine (2014 – 2019)

Project ID: TE02000058

(project of the Competence centre programme)

Co-investigator: Dr. Ing. Martin Palkovič

The primary objective of the Center of Competence for molecular diagnostics and personalized medicine, is to achieve a critical mass of experts, institutions, and knowledge in research, development, certification, technology transfer, and commercialization of in vitro diagnostics, in order to create a market oriented flexible national network in the area of diagnostic, prognostic and predictive biomarkers and to enable further development of personalized medicine.

INTERNATIONAL GRANTS

ANTAREX – AutoTuning and Adaptivity appRoach for Energy efficient eXascale HPC systems (2015 – 2018)

Project ID: 671623 (H2020-FETHPC-2014 call)

Co-investigator: Dr. Ing. Jan Martinovič

The main goal of the ANTAREX project is to provide a breakthrough approach to express by a Domain Specific Language the application self-adaptivity and to runtime manage and autotune applications for green and heterogeneous High Performance Computing systems up to the Exascale level.

www.antarex-project.eu

ExCAPE – Exascale Compound Activity Prediction Engine (2015 – 2018)

Project ID: 671555 (H2020-FETHPC-2014 call)

Co-investigator: Dr. Ing. Jan Martinovič

The main goal of the ExCAPE project is to develop an Exascale compound activity prediction engine by producing state of the art scalable algorithms and implementations suitable for running on future Exascale machines. Designed methods will enable processing and analysis of industry scale complex pharmaceutical analysis workloads.

www.excape-h2020.eu

READEX – Runtime Exploitation of Application Dynamism for Energy-efficient eXascale computing (2015 – 2018)

Project ID: 671657 (H2020-FETHPC-2014 call)

Co-investigator: Dr. Ing. Lubomír Říha

Supercomputers energy consumption is increasing in the approach to exascale. The main goal of the participating institutions is to develop an autotuning tool which would make computations and simulations more energy efficient by employing new scenarios and techniques changing software and hardware parameters such as frequency of computational cores. The task of IT4Innovations consists of evaluation of dynamism in HPC applications, manual tuning especially of FETI solvers based on domain decomposition, combining direct and iterative methods and evaluation and validation of developed tools, taking results of manual tuning as the baseline.

www.readex.eu

HARPA – Harnessing Performance Variability (2013 – 2016)

Project ID: 612069 (FP7-ICT-2013-10 call)

Co-investigator: Doc. Dr. Mgr. Vít Vondrák

We supported the project mainly by the HPC use case of the Floreon+ system, which was funded from the budget of the Moravian-Silesian Region. Users can benefit from new technologies developed for the Floreon+ system within the project HARPA. In particular the software upgrade HARPA-OS which offers better availability and cost-effectiveness of the computations, and a higher error resilience of the system.

www.harpa-project.eu

EXA2CT – Exascale Algorithms and Advanced Computational Techniques (2013 – 2016)

Project ID: 610741 (FP7-ICT-2013-10 call)

Co-investigator: Prof. Dr. Ing. Tomáš Kozubek

IT4Innovations was involved in the development and implementation of an iterative sparse linear solver using the FETI and Hybrid FETI domain decomposition methods and communication hiding or avoiding techniques. The outputs have been implemented in our in-house ESPRESO and PERMON libraries.

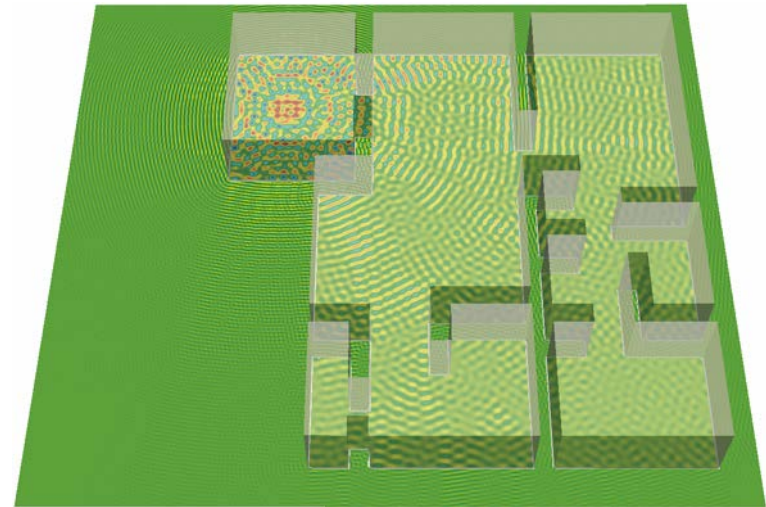
www.exa2ct.eu

Intel PCC – 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 will fund a group of scientists engaged in the development of algorithms and libraries for highly parallel machines. Algorithms will also be optimized for Intel's latest supercomputer technology.

ipcc.it4i.cz



Wave scattering transmission problem calculated using the library BEM4I. To prepare for the next generation of Intel Xeon Phi standalone processors, the library was also tested on Intel's Endeavour cluster providing access to the Knights Landing processors (KNL).

Collaboration with the commercial sector

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

In the framework of contractual research we cooperated with 11 companies and one university in 2016:

- PTS Josef Solnař, s.r.o.
- Continental Automotive
- LabControl s.r.o.
- K2 atmitec s.r.o.
- T-Mobile Czech Republic a.s.
- ITA, spol. s r.o.
- 3Dim Laboratory s.r.o.
- Triumf professional tools
- University of Ostrava
- VAKAR s.r.o.
- TESCANA Brno, s.r.o.
- The German Aerospace Center



Crash test simulations of new seats for improved passive safety and comfort of passengers in railway traffic, research project awarded the HiPEAC Technology Transfer Award



EDUCATIONAL AND TRAINING ACTIVITIES

EDUCATIONAL AND TRAINING ACTIVITIES

Study programme Computational Sciences

In the academic year 2016/2017, next to the running Doctoral programme Computational Sciences, we started also the Masters programme Computational Sciences. Within the scope of study, students can choose subjects as well as the theme of the diploma thesis from the following four specializations: data analysis and visualization, numerical parallel algorithms, computational physics and chemistry, and industrial applications. Two students enrolled in the Masters programme in 2016.

Eighteen students in total are enrolled in the Doctoral Study Programme Computational Sciences. In 2016, eight students started this course. The number of students in the doctoral programme thus increased by 44% compared to the previous year.

Students of the Masters Programme Computational Sciences can newly benefit from our collaboration with the Swiss university Università della Svizzera italiana. Thanks to the exchange programme, students can spend an entire semester at the prestigious Institute of Computational Sciences to extend their knowledge and skills.

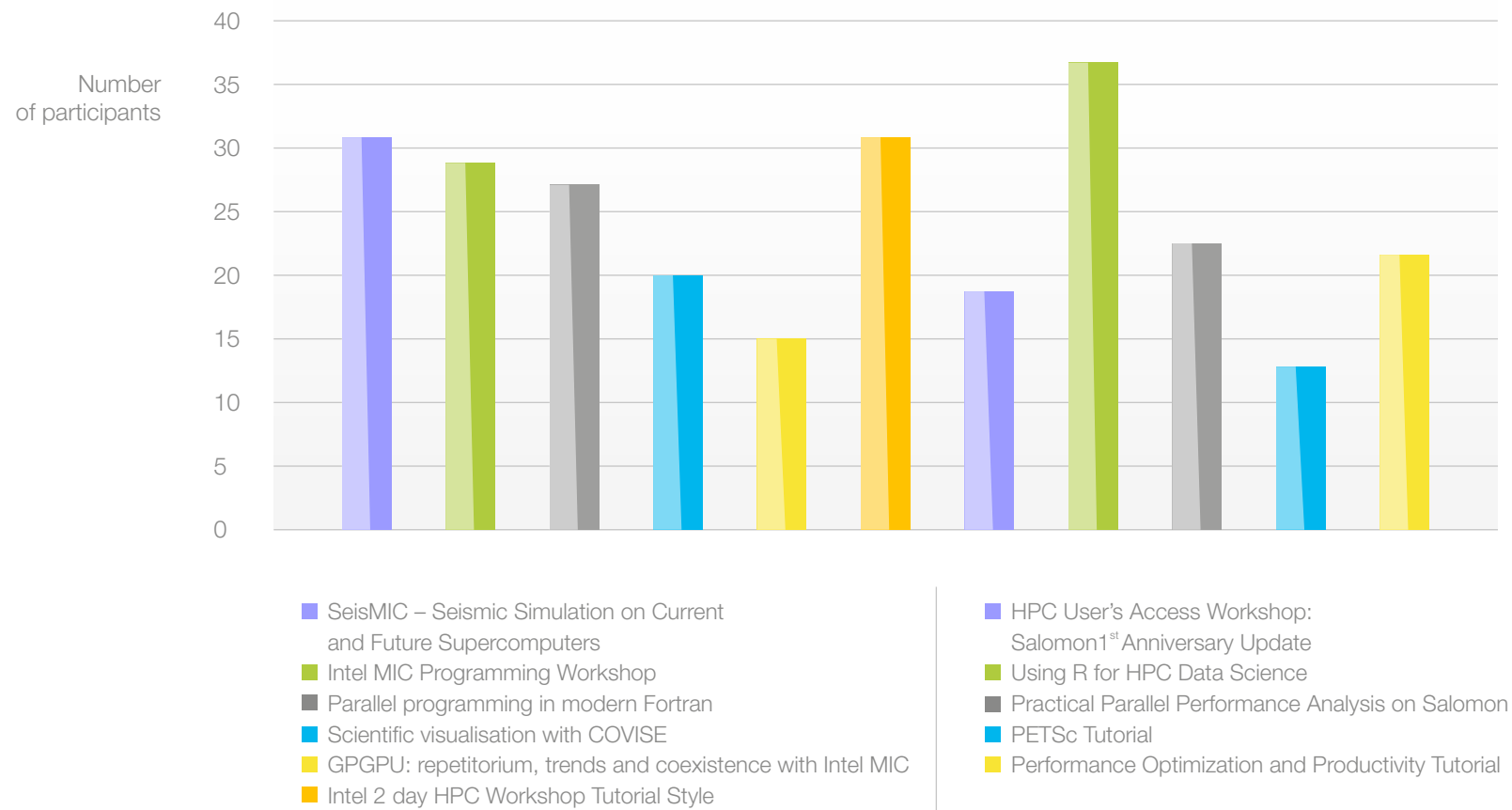
Educational activities

IT4Innovations supports the community of its users by offering high-quality technology courses, workshops and other educational activities. The primary goal of which is to broadly increase competency of users to efficiently utilize the unique computing systems of IT4Innovations. In the broader sense, we also aim to raise and increase awareness and the level of knowledge in the field of HPC nationwide in academia as well as the commercial and industrial sector.

The topics of these courses include computer systems and architectures, programming techniques, tools, libraries, and applications. In 2016 there were 11 training events held with a total of 267 participants. From those we would like to highlight several premium courses listed below:

- Parallel programming in modern Fortran (Salvatore Filippone, Cranfield University, UK)
- Scientific visualization with COVISE (Uwe Wössner, Martin Aumüller, High Performance Computing Center Stuttgart, Germany)
- Intel 2 day HPC Workshop Tutorial Style (Georg Zitzlsberger and Klaus-Dieter Oertel, Intel, Germany)
- Using R for HPC Data Science (George Ostrouchov, Oak Ridge National Laboratory and University of Tennessee, USA)

Training activities in 2016



Projects

INTERNATIONAL GRANTS

IPROCOM – The development of in silico process models for roll compaction (2013 - 2016)

Project ID: 316555 (FP7-PEOPLE-2012-ITN call)

Co-investigator: Prof. Dr. RNDr. Václav Snášel

IPROC

OM was a multidisciplinary and inter-sectoral consortium, the goal of which was to address scientific and technological challenges in the manufacture of particulate products (pharmaceuticals, fertilizers, biomass and metal components) through a coordinated and structured research training programme. IPROCOM brought together experts from the engineering, pharmaceutical science, materials science and computer science disciplines to provide structured training for the next generation of researchers.

IXPUG Workshop and Tutorials, March 2016

IT4Innovations
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supercomputing
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