



VSB TECHNICAL
UNIVERSITY
OF OSTRAVA

IT4INNOVATIONS
NATIONAL SUPERCOMPUTING
CENTER

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Managing Director's Introduction

Dear Readers,

We would like to present to you a review of the most important events and accomplishments that IT4Innovations National Supercomputing Center achieved in 2018. In this review, you can find information about our financial management, the amount of computational resources allocated within our Open Access Grant Competitions, the most important research results achieved, and interesting events held at our centre.

I am pleased that the demand for the computational resources of our supercomputers continues to grow. It demonstrates not only the increasing importance of supercomputing technologies in the research activities of our current users, but also the interest of brand-new users of our services. In the previous year, we distributed almost 172,000,000 core hours among 164 projects, while the excess of demand over the allocated amount was approximately 42 %. It was also one of the reasons for our pursuit of the procurement of a new cluster, which is to increase our current capacity. The contract with the economic operator was signed in November, and our users will have the new machine available in the first half of the year 2019.

Furthermore, we have been successful in the field of research and development. After having being nominated several times for the Best Poster Award at the most important conference dedicated to supercomputers – the Supercomputing Conference – our colleagues finally made it and won first place last year. We also achieved success in our endeavours in the field of international projects funded by the European Commission Horizon 2020 programme. In particular, the LEXIS project coordinated by our centre was approved for funding and its implementation is to commence in 2019.

During the year, we were also developing activities leading to more intensive collaboration with industry. In compliance with the upcoming Digital Europe and Digital Czech Republic programmes, we started to raise the profile of our Digital Innovation Hub in HPC and HPDA. We published the IT4Innovations Digital Innovation Hub brochure, which exemplifies our productive collaboration with industry. Building on it in the future, we would like to continue to increase our level of participation in the digitalization of industry and society alike.

This is only a brief summary of the many accomplishments achieved working together in 2018. The other important events can be found in the pages of this publication. I would like to express my thanks for its existence to our employees as well as our partners and supporters. Without them, we would not be able to review the past year with the joy and satisfaction resulting from good work done.



Vít Vondrák

Managing Director of IT4Innovations
National Supercomputing Center

IMPORTANT EVENTS IN 2018



In November 2018, we participated at the **Supercomputing Conference**, which is the world's largest gathering of scientists and companies operating in the field of high performance computing (HPC). It took place at the Kay Bailey Hutchison Convention Center in Dallas, Texas (USA) and was attended by more than 13 thousand participants. Our colleagues, Ondřej Meca, Lubomír Říha, and Tomáš Brzobohatý won the Best Poster Award for their contribution: Workflow for Parallel Processing of Sequential Mesh Databases. They won the competition over almost 100 posters, which were evaluated by the technical committee based on the quality of both the research work and presentation. It was our sixth time participating at this conference as an exhibitor.



At VSB - Technical University of Ostrava, an **agreement for the upgrade of HPC systems** for IT4Innovations National Supercomputing Center was signed on 9th November 2018. It includes extension of the Anselm cluster to a theoretical peak performance exceeding 800 TFlop/s (thus becoming 8 times more powerful than the currently operated system launched in 2013). This extension will be provided by Atos IT Solutions and Services, s.r.o.



In 2018, two achievements of our colleagues drew the attention of the European Commission, particularly its **Innovation Radar** Initiative. For the Innovation Radar Prize in the Excellent Research category, the HyperLoom software, which enables scientific and engineering pipelines of up to millions of interconnected computational tasks to be executed on a supercomputer, was nominated. In the Early Stage Innovation category, the intelligent online navigation system for citizens was nominated and shortlisted with three other finalists thanks to online voting. We have cooperated in the development of this system with the Sygic company with the objective to mitigate traffic congestion.



Since the beginning and the second half of the year 2018, we have been participating in the preparation and implementation of the **EuroHPC** Joint Undertaking, respectively. Within the collaboration of European countries, its objective is to support the path to building a European exascale supercomputer, and thus significantly contribute to digitalization of the European community and industry. In cooperation with the Ministry of Education, Youth and Sports of the Czech Republic and the European Commission, we organized a workshop dedicated to the EuroHPC initiative. The objective of this workshop was to allow representatives of the Czech research community and commercial sector to actively participate in discussing ways of implementing the EuroHPC initiative in the Czech Republic.



Since December 2018, we have been an Information Security Management System certificate holder according to the international **ISO 27001** (ISO/IEC 27001:2013, ČSN ISO/IEC 27001:2014) standard. The ISO 27001 certificate has been awarded for provision of national supercomputing infrastructure services, high-performance computing problem solutions, performance of advanced data analysis and simulations, and processing of large data sets. The awarded certification demonstrates that we continually improve the internationally recognized Information Security Management System, manage risks, have processes and policies in place to maximize information security to prevent its abuse, unauthorized modification, or loss.



We produced a new publication, **IT4Innovations Digital Innovation Hub**, where you can learn about particular examples of our cooperation with industry. Moreover, you can find there our portfolio of services including, for example, computationally intensive modelling and simulations, advanced data analysis, application of artificial intelligence methods, development and implementation of FEM/BEM simulation tools, assistance with deployment of codes on HPC systems, rendering, as well as renting of computational resources. You can learn about 19 particular examples of our collaboration with private enterprises based in mechanical engineering, the energy industry, the automotive industry, water management, the healthcare sector, geoinformatics, and others.

IMPORTANT EVENTS IN 2018



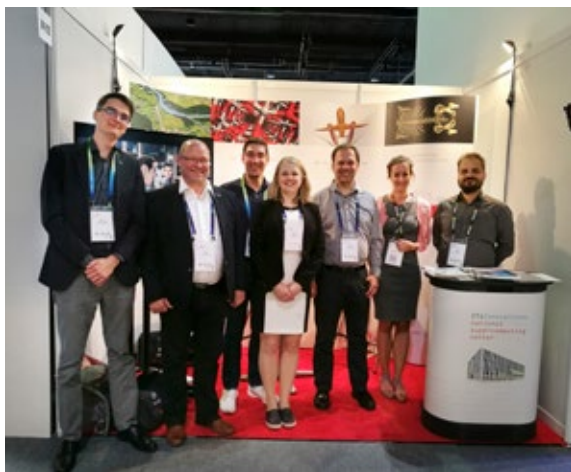
In 2018, we hosted the 3rd Day of **National Research Infrastructures**. Nearly 100 people from all over the Czech Republic gathered to participate in technical discussions on crucial current issues in policy making and funding of large research infrastructures in the Czech Republic. Lukáš Levák, the director of the Department for Research and Development of the Ministry of Education, Youth and Sports made an appearance at the conference, where he presented the Research Infrastructures financial framework for the years 2020–2022. We also organized the **2nd IT4Innovations Users Conference**. We hosted almost 100 attendees, who had an opportunity to listen to contributions from various scientific domains and exchange their user experience. The conference programme included 20 talks as well as a poster section for presentation of research projects.



In 2018, we hosted the prestigious International **HPC Summer School on Challenges in Computational Sciences**, IHPCSS, with the participation of nearly 80 students and 30 mentors from Europe, the United States of America, Canada, and Japan.



Already for the sixth time, the **Summer of HPC** programme has offered students of European universities summer internships focused on HPC in the countries participating in the Partnership for Advanced Computing in Europe (PRACE) project. This summer, 23 students were given the opportunity to participate in summer internships at 11 host organizations. Two of these students were welcomed at IT4Innovations.



It has already been the fifth time that we have presented our infrastructure and research to the visitors of the largest European HPC focused event – the **International Supercomputing Conference**, which attracts more than 3,000 experts and students from all over the world every year.



Events aimed at the general public held at our centre last year attracted more than 1,700 visitors. These events included, for example, excursions for pupils, students, and companies, and popularisation events such as Researchers's Night. We have already for the second time presented our infrastructure and research at the NATO Days in Ostrava, which attracted 220,000 visitors in 2018.



In 2018, we organized **12 educational and training courses**, which were attended by nearly 240 participants altogether.

IT4INNOVATIONS PROFILE

IT4Innovations National Supercomputing Center at VSB – Technical University of Ostrava (hereinafter referred to as IT4Innovations) represents a strategic large research infrastructure in the Czech Republic, and together with other two infrastructures, CESNET and CERIT-SC, constitutes the E-infrastructure of the Czech Republic. The National Supercomputing Center provides state-of-the-art supercomputing technology and services and conducts excellent research in the field of high performance computing (HPC) and data analysis (HPDA).

Mission

Our mission is to carry out excellent research in the field of high performance computing and advanced data analysis, and to operate the leading national supercomputing infrastructure, mediating its effective use in order to increase the competitiveness and innovation of Czech science and industry.

Vision

Our vision is to become a leading supercomputing centre that provides professional services and conducts excellent research in the field of high-performance computing and processing of advanced data sets for the benefit of science, industry, and the whole of society.

Since 2011, IT4Innovations has been a member of the 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, IT4Innovations became a member of the European Technological Platform for HPC (ETP4HPC), which is focused, amongst other things, on defining research priorities in the field of supercomputing. The main research areas of IT4Innovations include big data processing and analysis, development of parallel scalable algorithms and libraries, supercomputing technology development, solution of computationally demanding engineering problems, and modelling for nanotechnologies and materials research.

For the Czech scientific community, IT4Innovations provides access to high-performance computing systems and a wide range of training sessions aimed at acquiring the knowledge needed to efficiently use our supercomputing infrastructure. Furthermore, IT4Innovations cares 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.

Given the gradual development of IT4Innovations as well as the demands of the Czech and European research communities, and the whole of society, we decided to update our mission and vision for the period 2018 to 2020.



Also in 2018, IT4Innovations continued in its collaboration with the partners of the IT4Innovations Centre of Excellence project – namely 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. Supervision of this project as well as the sustainability of the original Centre of Excellence project is ensured by the Supervisory Board.

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

CHAIRMAN:

Doc. Vít Vondrák

MEMBERS:

Prof. Michael Čada
Prof. Jean-Christophe Desplat
Prof. Petr Berka
Prof. Peter Arbenz
Doc. Petr Cintula
Prof. Ulrich Bodenhofer
Prof. Kenneth Ruud
Prof. Arndt Bode
Prof. Roman Wyrzykowski

**Scientific Council of
IT4Innovations, University
Institute of VSB – Technical
University of Ostrava**

CHAIRMAN:

Doc. Vít Vondrák

MEMBERS:

Dr Branislav Janský
Dr Jan Martinovič
Prof. Tomáš Kozubek
Prof. Jaromír Pištora
Prof. Miroslav Vozňák
Prof. Jan Holub
Prof. Pavel Tvrdík
Doc. Stanislav Hledík
Prof. Jaroslav Pokorný
Doc. Jiří Jaroš
Dr Tomáš Karásek
Dr Lubomír Říha

Supervisory Board

CHAIRMAN:

Evžen Tošenovský, Dr.h.c.

VICE-CHAIRMAN:

Doc. Pavel Drozd

MEMBERS:

Prof. Ivo Vondrák
Prof. Petr Noskievič
Miroslav Murin, FCCA
Prof. Pavel Zemčík
Leoš Dvořák
Doc. Pavel Tuleja
Prof. Miroslav Tůma

ADMINISTRATIVE AND FINANCIAL REVIEW

Management of IT4Innovations



Radim Mrázek

Administration and Finance



Tomáš Kozubek

Research and Development



Branislav Janský

Supercomputing Services

Employees of IT4Innovations

Employees of IT4Innovations by divisions in full time equivalent (FTE), 143.43 FTE in total:



21 %

**Management and
Administration**



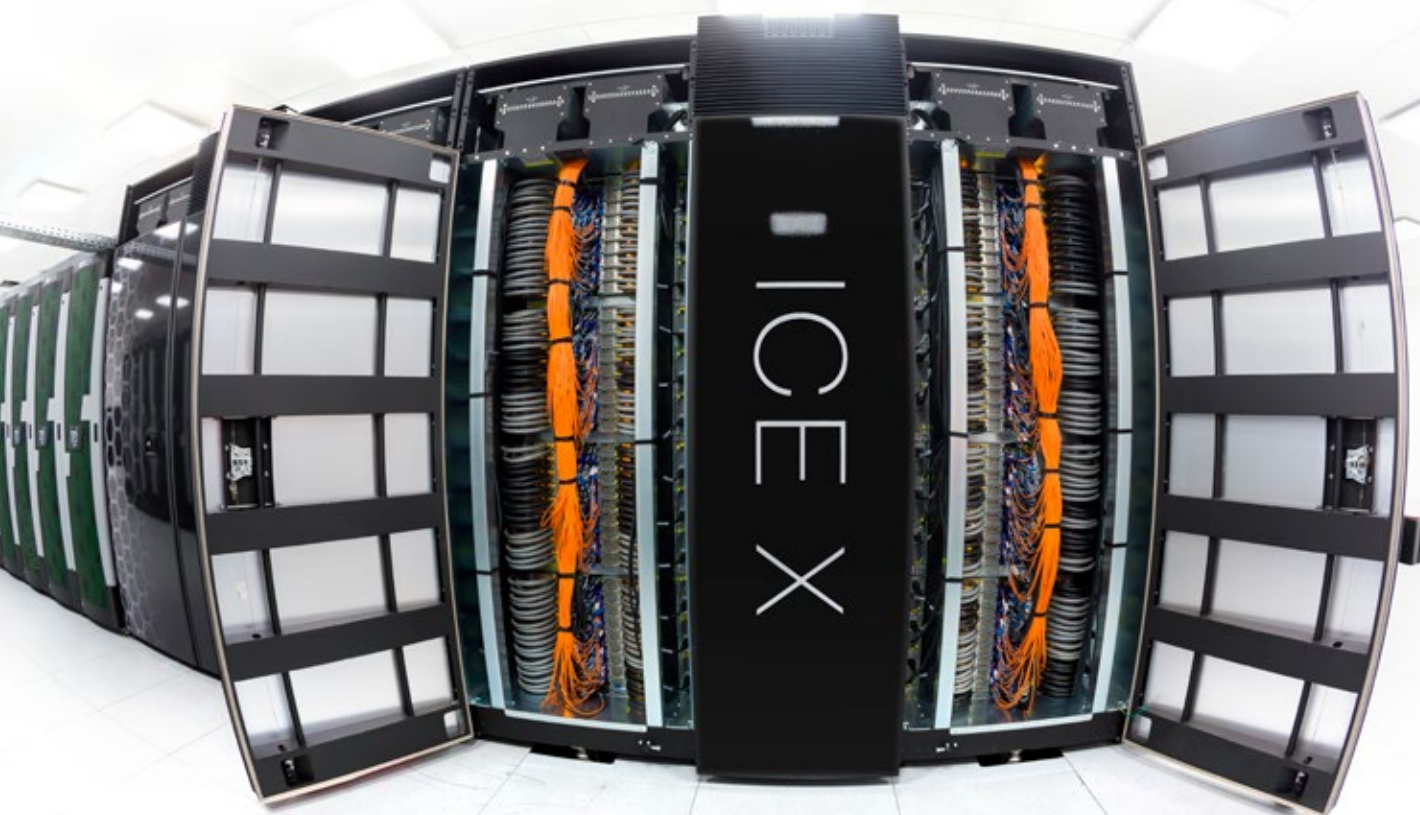
69 %

**Research and
Development**

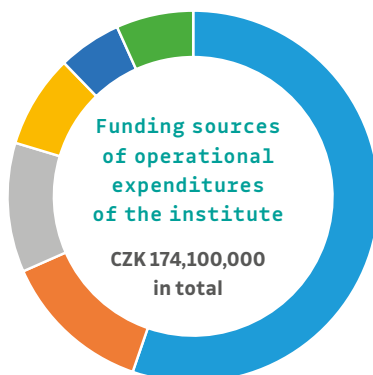


10 %

**Supercomputing
Services**



Sources of Funding

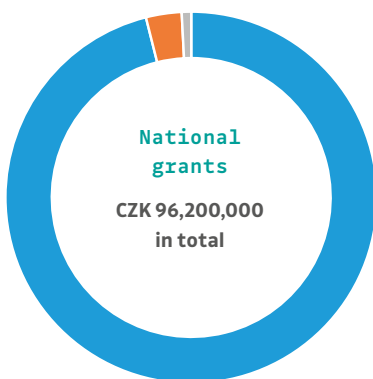


- 55.3 % National grants
- 13.1 % Operational Programme Research, Development and Education
- 11.3 % International grants
- 8.1 % Institutional support
- 5.5 % Contract research and rental of computational resources
- 6.7 % Others

In 2018, the overall budget of IT4Innovations was CZK 174,100,000. The largest share of the funding sources for operational expenses of the institute was contributed by national grants (55.3 %). Other funding sources for operational expenses of the institute included Operational Programme Research, Development and Education (13.1 %), international grants (11.3 %), institutional support (8.1 %), and contract research together with renting out computational resources (5.5 %). Other sources of funding (6.7 %) include mainly the Operating fund.



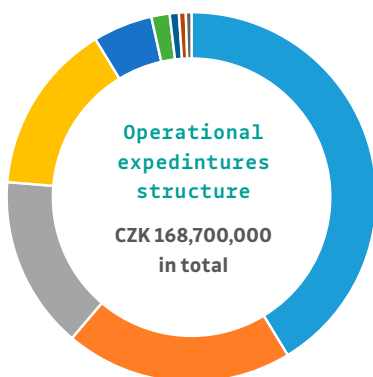
- 18.8 % ExCAPE
- 17.4 % ANTAREX
- 16.3 % READEX
- 15.1 % PRACE, 5th implementation phase
- 7.2 % InnoHPC
- 7.1 % CloudiFacturing
- 6.1 % EXPERTISE
- 4.4 % IPROCOT (grant settlement)
- 3.2 % LOWBRASYS
- 2.6 % TETRAMAX
- 1.0 % ExaQute
- 0.7 % POP2
- 0.2 % Superheroes 4 Science



- 96.1 % Ministry of Education, Youth and Sports of the Czech Republic (16 projects)
- 3.1 % Technology Agency of the Czech Republic (2 projects)
- 0.8 % Grant Agency of the Czech Republic (1 project)

Operational and Capital Expenditures

The total expenditures of IT4Innovations amounted to CZK 174,100,000. Within this amount, non-investment (operational) expenses and investment (capital) expenses amounted to CZK 168,700,000 and CZK 5,400,000, which is 96.9 % and 3.1 %, respectively. The largest part of operational expenses included personnel expenses, services, and overhead expenses (91.3 %).



- **41.3 %** Personnel expenses - research teams
- **19.9 %** Personnel expenses - management administration, and supercomputing services
- **15.1 %** Services
- **15.0 %** Overhead expenses
- **5.2 %** International and domestic business trips (including those of invited speakers)
- **1.6 %** Fees
- **0.8 %** Scholarships
- **0.6 %** Consumables
- **0.5 %** Small tangible fixed assets



Summary of All Grants

National Grants

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

Large Infrastructures Project for Research, Experimental Development, and Innovation

- IT4Innovations National Supercomputing Center

National Programme of Sustainability II

- IT4Innovations Excellence in Science

Grants for specific university research for 2018

- Optimization of Machine-learning Algorithms for an HPC Platform
- Dynamic Systems Problems and their Implementation on HPC

- Hardware Acceleration of Matrix Assembler and GUI Development of ESPRESO Library
- Development of Tools for HPC Applications Energy Optimization
- Solving Problems with Uncertainties Using the Boundary Element Method
- Internationalization of Doctoral Education in Molecular Physics
- Application of Topology Optimization Methods in Engineering Practice
- Hydroxyapatite Nanocomposites: Structure and Modelling
- Modelling of Diffractive and Plasmonic Nanostructures
- Elipsometry and Magneto-optical Properties of Pr and Nd Based Perovskites and MO Effect in Cubic (011) Oriented Transition Metals Layers on MgO Substrate

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

Researcher Mobility support within international cooperation in R&D&I

- **NEW** Modeling of Interactions of Cold Rare-gas Plasmas with Ambient Air
- **NEW** Metal-graphene Interfaces – Foundations of Novel Spintronic Materials
- **NEW** Understanding of the Magnetostriction in Fe-Ti Alloys by First-principles Calculations

Projects supported by the Grant Agency of the Czech Republic

- Novel Fuel Materials for the IV Generation Nuclear Reactors

SUPERCOMPUTING
SERVICES

RESEARCH AND
DEVELOPMENT

EDUCATIONAL AND
TRAINING ACTIVITIES

**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

**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 Education Training Center
- Technology for the Future
- Artificial Intelligence and Reasoning
- **NEW** Science without Borders

**International
Grants**

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

- PRACE-5IP – Partnership for Advanced Computing in Europe, 5th Implementation Phase
- 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
- **NEW** ExaQute – Exascale Quantifications of Uncertainties for Technology and Science Simulation
- **NEW** POP2 – Performance Optimisation and Productivity 2

**Project of the Interreg
Danube Transnational
Programme (EU funds)**

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

**International
Visegrad Fund**

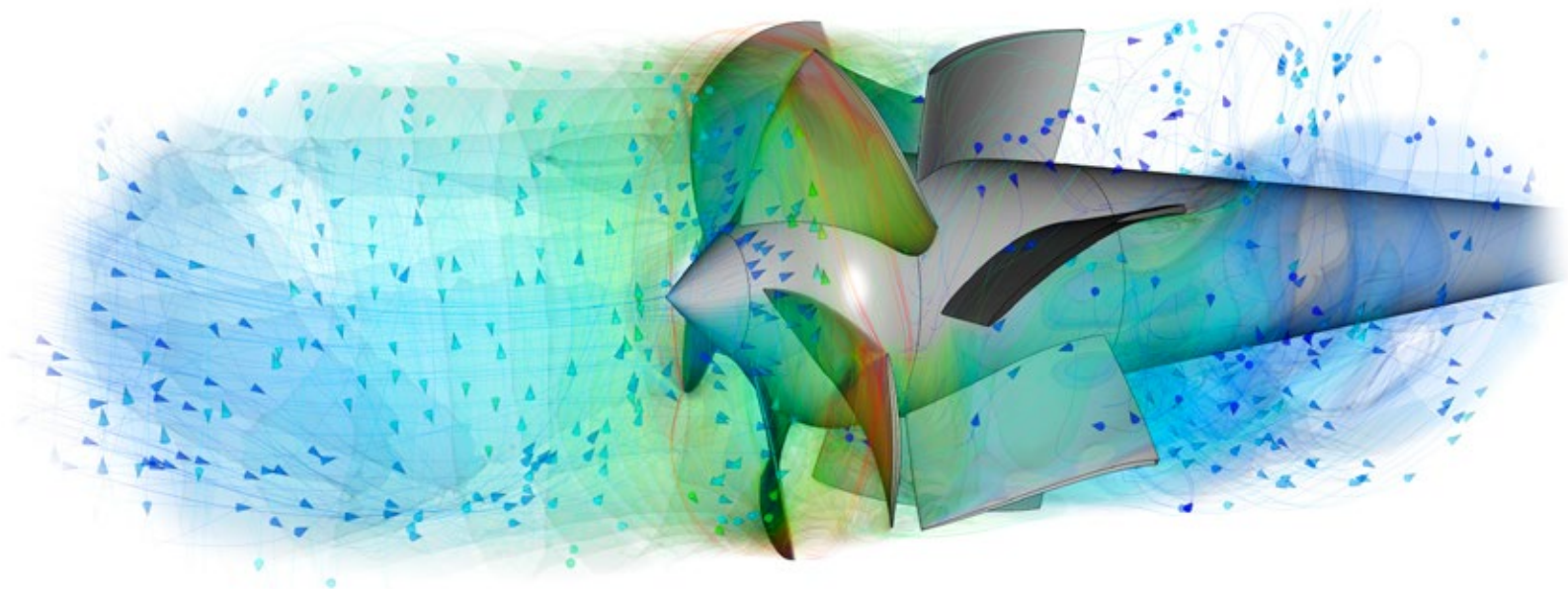
- **NEW** Superheroes 4 Science

SUPERCOMPUTING SERVICES

IT4Innovations 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.

In 2018, selection procedures were launched to modernize the **IT4Innovations supercomputing infrastructure within the IT4Innovations National Supercomputing Center - Path to Exascale** project funded by Operational Programme Research, Development and Education of the Ministry of Education, Youth and Sports of the Czech Republic. These selection procedures will result in an increase in the IT4Innovations su-

percomputing infrastructure capacity in 2019, including a computer cluster delivering a performance of more than 800 TFlop/s and equipped with the latest available technologies, the NVIDIA DGX-2 system, centralised ICT infrastructure with a project storage and WAN, and virtualization infrastructure. In 2020, further significant extension of our computing systems is expected to meet our users' needs.



Technical Specifications of the Supercomputers

213th on the TOP500
list of the most powerful
supercomputers
in the world

November 2018

REVIEW
2018

	ANSELM	SALOMON
Put into operation	Spring 2013	Summer 2015
Theoretical peak performance	94 TFlop/s	2,011 TFlop/s
Operating system	RedHat Linux 64bit 6.x	RedHat Linux 64bit 6.x CentOS 64bit 6.x
Compute nodes	209	1,008
CPU	2x Intel SandyBridge 8 cores, 2.3 / 2.4 GHz 3,344 cores in total	2x Intel Haswell 12 cores, 2.5 GHz 24,192 cores in total
RAM per compute node	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 52,704 cores in total
Storage	320 TiB /home (2 GB/s) 146 TiB /scratch (6 GB/s)	500 TiB /home (6 GB/s) 1,638 TiB /scratch (30 GB/s)
Interconnection	Infiniband QDR 40 Gb/s	Infiniband FDR 56 Gb/s

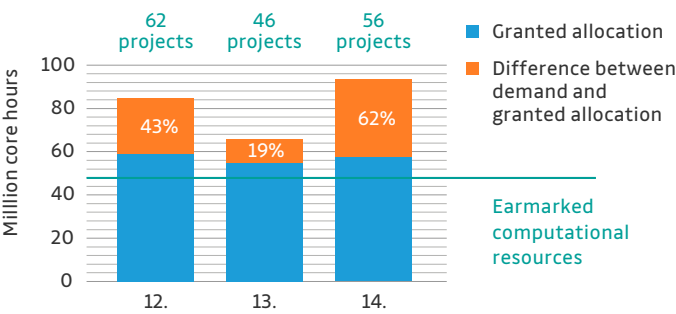
Computational Resources Allocation

The computational resources of IT4Innovations are dedicated to 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.

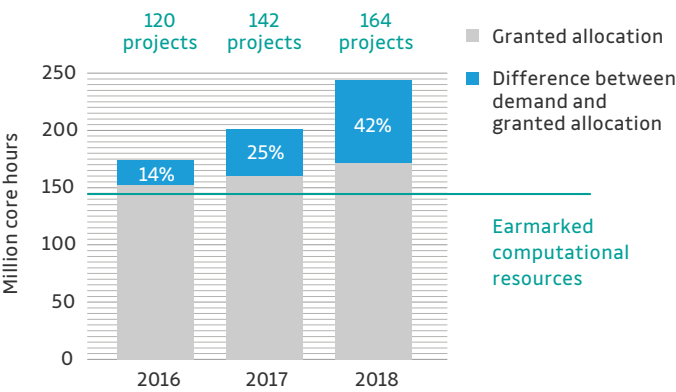
Institutions can apply for computational resources within Open Access Grant Competitions. These are announced three times a year. In 2018, almost 172 million core hours were allocated within three Open Access Grant Competitions, and distributed among 164 research projects, enhancing Czech science.

The computational resources earmarked for an Open Access Grant Competition amount to 48 million core hours. In 2016 and in 2017, the excess demand for core hours over the available capacity amounted to almost 21 % and more than 39 %, respectively. In contrast, in 2018 it was almost 70 %. 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. The difference between the core hours demand and the computational resources reserved for Open Access Grant Competitions is compensated by the reserves available through the Directors' Discretion scheme as well as the Anselm system computational resources. In 2018, the difference between the demand and the allocated amount was about 42 %.

Open Access Grant Competitions in 2018



Comparison of the demand and allocated computational resources within Open Access Grant Competitions in 2016-2018



Year	Difference between demand and earmarked computational resources (3*48 million corehours)	Difference between demand and granted allocation
2016	21 %	14 %
2017	40 %	25 %
2018	70 %	42 %

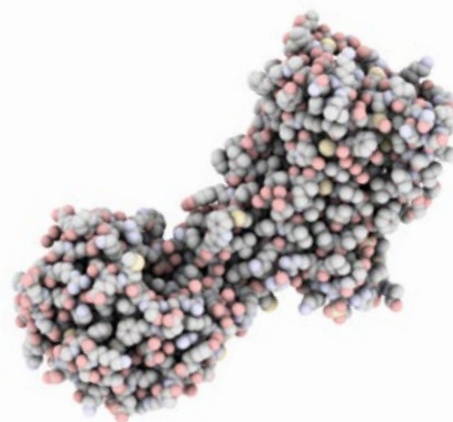
Within the Open Access Grant Competitions in 2018, a total of 42 projects of applicants from VSB – Technical University of Ostrava were awarded the computational resources amounting to approximately 43 million core hours. Nine projects were led by researchers from the Faculty of Civil Engineering, the Faculty of Electrical Engineering and Computer Science, the Nanotechnology Centre, the Faculty of Mechanical Engineering, and the Faculty of Materials Science and Technology. The remaining 33 projects were led by researchers from IT4Innovations, a university institute of VSB-TUO.



Results of the 12th Open Access Grant Competition in Q1/2018 Newsletter

Concerning the external research institutions using the IT4Innovations infrastructure, most of the computational resources were allocated for the projects of researchers affiliated with the Czech Academy of Sciences (CAS). Their 10 institutes were allocated 38.5 million core hours for a total of 31 projects. Most of the computational resources were allocated to the projects of the Institute of Organic Chemistry and Biochemistry, and the J. Heyrovsky Institute of Physical Chemistry.

Almost 10 million core hours or more were also awarded to other institutes as well, namely CEITEC, Charles University, the Czech Technical University in Prague (CTU in Prague), and Masaryk University.



Reconstruction of encephalitis virus using cryo-electron microscopy and the project of Dr Pavel Plevka from CEITEC MU

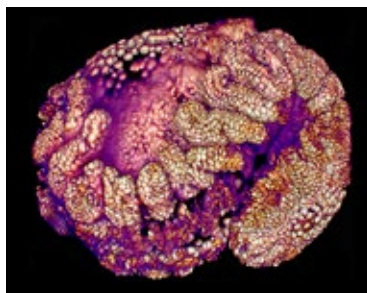
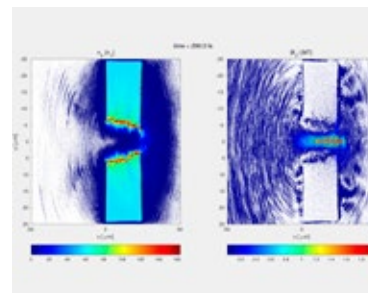


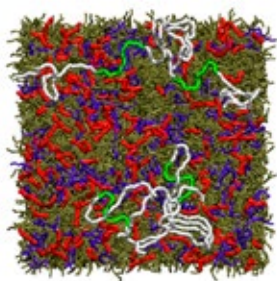
Image of the Crustacean (Parhyale) embryo imaged by light sheet microscope and the project of Dr Pavel Tomančák from IT4Innovations



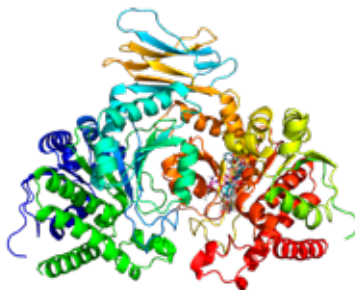
2D simulation results visualization of a laser pulse interaction and the project of Martin Matys from CTU in Prague



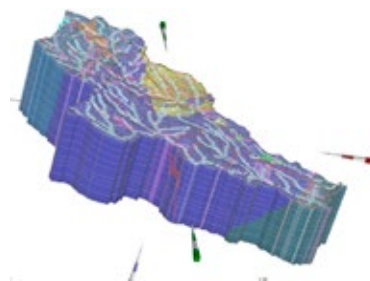
Results of the 13th
Open Access Grant Competition
in Q2/2018 Newsletter



Simulations of the interaction of
human tear film with drugs and the
project of Dr Lukasz Cwiklik from the
Czech Academy of Sciences



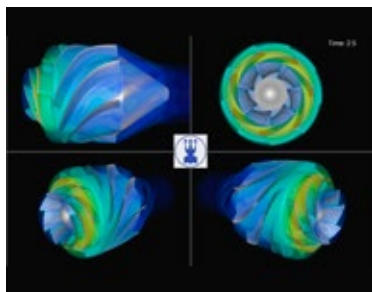
Inhibitor molecule bound in the active
area of isocitrate dehydrogenase
1 enzyme (idh1) and the project of
Dr Gaspar Pinto and Jan Štourač from
Masaryk University



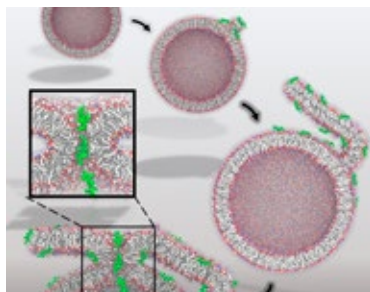
Geological model (FEFLOW) and the
project of Dr Michal Podhorányi from
IT4Innovations



Results of the 14th
Open Access Grant Competition
in Q4/2018 Newsletter



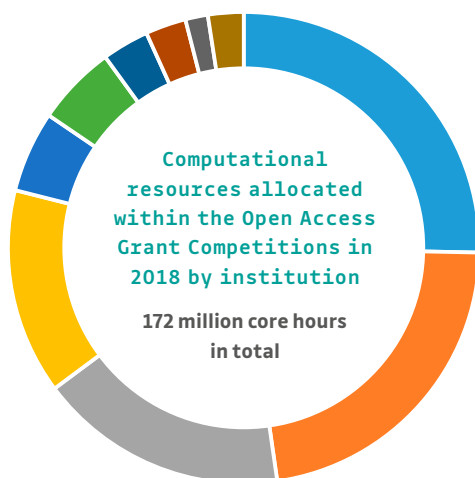
CFD simulation of water pump
and the project of Tomáš Krátký
from Palacký University



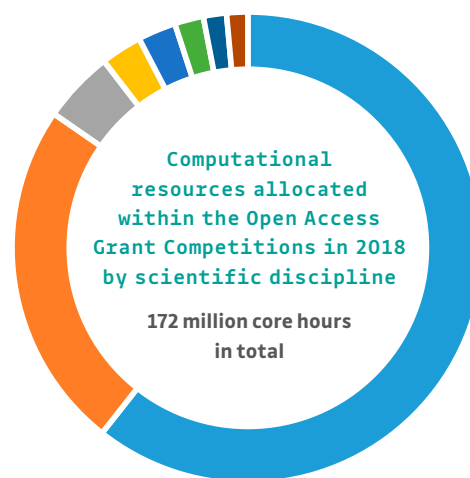
Cell-penetrating peptide and the
project of Prof. Pavel Jungwirth from
the Czech Academy of Sciences



Virtual screening of libraries and
the project of Prof. Pavel Hobza from
the Czech Academy of Sciences



- 25 % VSB – Technical University of Ostrava (42 projects)
- 22 % Czech Academy of Sciences institutes (31 projects)
- 17 % CEITEC (10 projects)
- 14 % Charles University (36 projects)
- 6 % The Czech Technical University in Prague (8 projects)
- 6 % Masaryk University (9 projects)
- 3 % Brno University of Technology (8 projects)
- 3 % The University of Ostrava (5 projects)
- 2 % Tomáš Baťa University in Zlín (3 projects)
- 2 % Others (12 projects)



- 61 % Material sciences (48 projects)
- 24 % Biosciences (32 projects)
- 5 % Engineering (25 projects)
- 3 % Physics (9 projects)
- 3 % Earth sciences (20 projects)
- 2 % Applied mathematics (16 projects)
- 1 % Computational sciences (8 projects)
- 1 % Astrophysics (6 projects)

The lists of projects awarded computational resources within the Open Access Grant Competitions in 2018, in the order 12th, 13th, and 14th Open Access Grant Competition



12

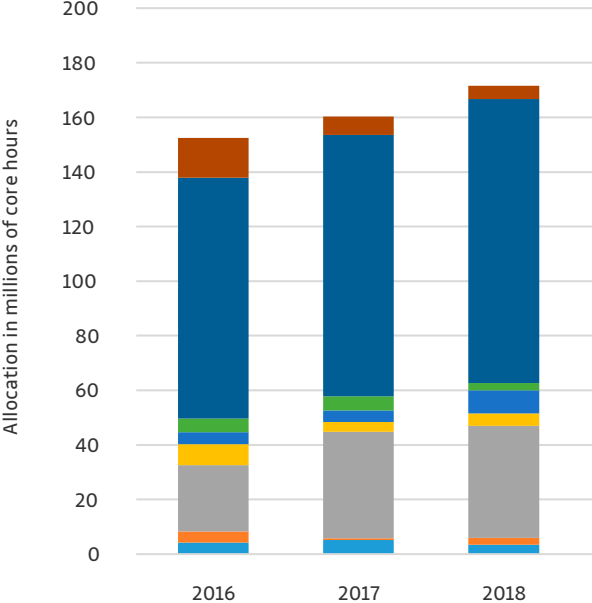


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14

In the last three years, almost 490 million core hours were distributed among 426 projects within Open Access Grant Competitions. 81 % of the computational resources were awarded to projects focused on material sciences and biosciences.

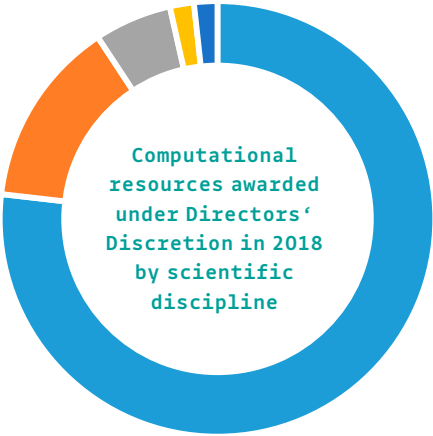


Allocation of computational resources in 2016, 2017, and 2018 by scientific discipline

- Physics (30 projects)
- Material sciences (124 projects)
- Computational sciences (34 projects)
- Engineering (60 projects)
- Earth sciences (44 projects)
- Biosciences (88 projects)
- Astrophysics (9 projects)
- Applied mathematics (37 projects)

Furthermore, 5 % of the IT4Innovations computational resources can also be granted to projects upon request within the Directors' Discretion scheme. An application can be submitted at any time. The computational resources are allocated irregularly based on 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 Directors' Discretion scheme in 2018, a total of 17 projects were allocated 4 million core hours.

Private enterprises have the opportunity to rent the computational resources. In 2018, 7 enterprises concluded rental agreements, the total amount of which was about 3 million core hours.



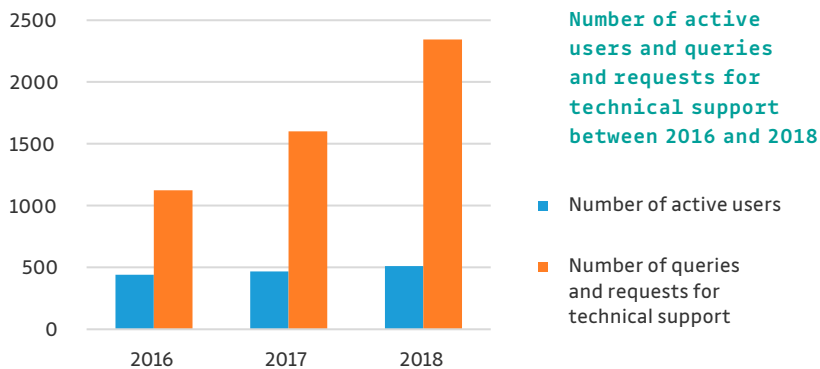
- 77 % Material sciences (2 projects)
- 14 % Engineering (6 projects)
- 6 % Biosciences (3 projects)
- 2 % Computational sciences (3 projects)
- 1 % Applied mathematics and Earth sciences (3 projects)

Users of Computational Resources

In 2018, the number of active users was 510 in total. In comparison with 2017, this has increased by 8.7 %.

In 2018, the IT4Innovations Technical Support received 2,343 queries and requests of which 2,341 were solved successfully, and 2 were rejected.

The internal response time (24 h for the first response) was observed in 99.96 % of queries. The internal closure time, which should not be longer than 30 days, was observed in 99.23 % of queries.



Projects

Several national and international grants help IT4Innovations secure operation and development of its supercomputing infrastructure. In terms of operation of the current systems, the most important one is the grant from the Ministry of Education, Youth and Sports of the Czech Republic (MEYS) – **IT4Innovations National Supercomputing Center**, which is funded by sources dedicated to supporting Large Infrastructures for Research, Experimental Development, and Innovation. Modernization of the IT4Innovations computational capacity is

funded by the Operational Programme Research, Development, and Education of MEYS, in particular, by the **IT4Innovations National Supercomputing Center – Path to Exascale project**. The important international projects we are involved in thanks to our participation in the Partnership for Advanced Computing in Europe (PRACE) include the eponymous infrastructure projects funded by the European Commission Horizon 2020 programme. In 2018, the 5th implementation phase of the project titled PRACE-5IP was implemented.

National Grants

IT4Innovations National Supercomputing Center (2016–2019)

PROJECT ID LM2015070 (Large Infrastructures for Research and Experimental Development and Innovations project)

PRINCIPAL INVESTIGATOR

Doc. 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 a system with a theoretical peak performance of 2 PFlop/s, and a smaller system with theoretical peak performance of 94 TFlop/s.

Necessary for providing the aforementioned computing capacities is the operation of the related infrastructure (power supply, cooling, safety, fire protection, etc.), as well as user support and the management of computing and infrastructure systems. In addition, research activities that streamline its operation and extend its use to the user are also part of the project. The educational and training activities that are open to the broader scientific community of the Czech Republic also contribute to effective use of the infrastructure.

www.msmt.cz



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 Infrastructure)

PRINCIPAL INVESTIGATOR

Dr Branislav Jansik

The objective of this project is to upgrade and modernize the research infrastructure of IT4Innovations so as to at the very least 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 equipment and supplementing the current Anselm supercomputer with a similar modern supercomputer (Small cluster) in terms of extent and function in 2018. In 2020, a new supercomputer, exceeding the capacity of Salomon, the most powerful system of IT4Innovations so far, is to be procured.

Additional objectives of the project also include the support of high-quality research across the wider academic community in the Czech Republic, and the expansion of existing research activities at 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 the services provided by this infrastructure to its users.

International Grants

PRACE-5IP – Partnership for
Advanced Computing in Europe,
5th implementation phase
(2017–2019)

PROJECT ID 730913
(H2020-EINFRA-2016-1 Call)

PRINCIPAL INVESTIGATOR

Doc. Vít Vondrák

The objectives of the PRACE (Partnership For Advanced Computing in Europe) projects are to build on the 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.

www.prace-ri.eu/prace-5ip/

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 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.

www.interreg-danube.eu



RESEARCH AND DEVELOPMENT

The key IT4Innovations research topics are related to the use of the supercomputing infrastructure such as advanced data processing and analysis, application of artificial intelligence methods, parallel scalable algorithms development, solving challenging engineering problems, modelling for nanotechnologies and materials research, and supercomputing infrastructure research. The research in these areas is concentrated

into 5 laboratories. The Parallel Algorithms Research Lab is focused on developing its own in-house scalable algorithms and software libraries, which are used for collaboration with both academic and industrial partners. The Advanced Data Analysis and Simulations Lab is focused on big data processing and analysis that are part of advanced data-based computer simulations. The Modelling for Nanotechnologies Lab is

focused on designing novel materials using electronic structure calculations. The Big Data Analysis Lab is focused on uncovering information hidden in large data sets. In January 2017, the Infrastructure Research Lab was also newly established. This lab has enhanced our own in-house infrastructure research and is focused on developing methods for innovative use, operation, and monitoring of the computing infrastructure.

Lab	Acronym	Head of Lab	FTE
Parallel Algorithms Research Lab	PAR	Dr Tomáš Karásek	22.25
Advanced Data Analysis and Simulations Lab	ADAS	Dr Jan Martinovič	35.43
Modelling for Nanotechnologies Lab	NANO	Prof. Jaromír Pištora	20.13
Big Data Analysis Lab	BIGDATA	Prof. Miroslav Vozňák	6.34
Infrastructure Research Lab	INFRA	Dr Lubomír Říha	14.40

Throughout the year 2018, the Research Council of the IT4Innovations Centre of Excellence evaluated six project proposals for the main research areas representing IT4Innovations scientific excellence. The IT4Innovations flagships include three project proposals:

ESPRESSO, a highly parallel solver library for engineering applications

PRINCIPAL INVESTIGATOR Dr Tomáš Brzobohatý

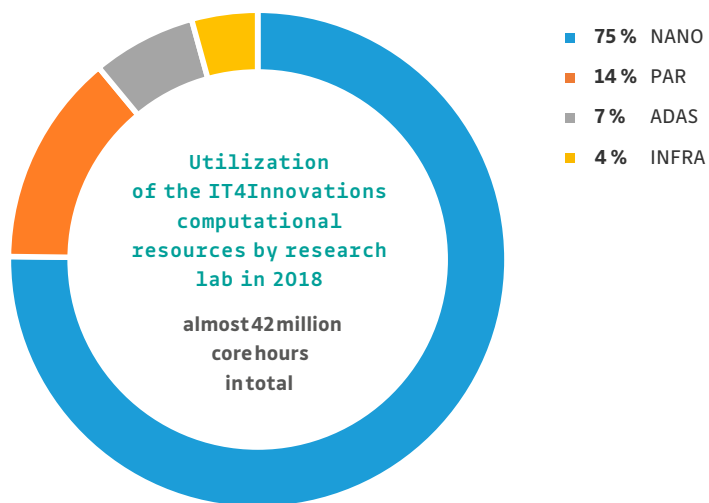
Materials design – closer to reality using exascale computing

PRINCIPAL INVESTIGATOR Dr Dominik Legut

HPC platforms for scientific workflow execution

PRINCIPAL INVESTIGATORS Dr Jan Martinovič, and Dr Stanislav Böhm

In 2018, almost 42 million core hours, 24 % of the total allocated amount, were distributed among 33 projects of the IT4Innovations research laboratories within the Open Access Grant Competitions. The Parallel Algorithms Research Lab submitted the most projects whereas the largest share of the computational resources was awarded to the Modelling for Nanotechnologies Lab.



Significant events

- > The **Best Poster Award** for the paper “Workflow for Parallel Processing of Sequential Mesh Databases” at the Supercomputing Conference, November 2018, Dallas, USA.
- > Funding approved for the H2020 ExaQUTE (Exascale Quantifications of Uncertainties for Technology and Science Simulation) project. The project started in June 2018 and its main objective is to develop new methods for solving complex engineering problems using numerical simulations and future exascale systems.
- > Successful cooperation with the University of Toulouse in PhD students education; 1 successfully defended their thesis before a Czech-French committee (Cyril Van de Steen, Modelling of Transport Properties of Ions of Krypton and Xenon for Optimization of Cold Rare-gas Plasmas Generators); 1 new student within the cotutelle programme (Martin Beseda, Modelling of Transport Properties of Molecular Ions of Helium in Air); the award of funding for another student.
- > Contract research amounting to more than CZK 2 million with companies such as Continental Automotive Czech Republic s.r.o., Invent Medical Group s.r.o., Borcad cz s.r.o., Doosan Škoda Power, s.r.o., and Siemens s.r.o.

Selected publications

- > Brzobohatý, T., M. Jarošová, R. Kučera, V. Šátek. Path-following Interior Point Method: Theory and Applications for the Stokes Flow with a Stick-slip Boundary Condition. *Advances in Engineering Software*. 2018. DOI: 10.1016/j.advengsoft.2018.06.010. Q1, IF=3,198.
- > Van de Steen, C., M. Benhenni, R. Kalus, B. Lepetit, F. X. Gádea, M. Yousfi. Quantum and Semi-classical Collision Cross-sections and Transport Data for Kr⁺/Kr system. *Plasma Sources Science and Technology*. 2018, 27(6). DOI: 10.1088/1361-6595/aac8c1. Q1, IF=3,302.
- > Ćosić R., A. Vítek, R. Kalus. Photoabsorption Spectra of Small Mercury Clusters. A computational study. *Physical Chemistry Chemical Physics*. 2018, 20(45). DOI: 10.1039/C8CP04858D. Q2, IF=3,906.

- > Zapoměl, J., P. Ferfecki. The Oscillation Attenuation of an Accelerating Jeffcott Rotor Damped by Magnetorheological Dampers Affected by the Delayed Yielding Phenomenon in the Lubricating Oil. *Journal of Vibration and Acoustics*. 2018, 140 (1). DOI: 10.1115/1.4037512. Q2, IF=1,777.
- > Říha L., M. Merta, R. Vavřík, T. Brzobohatý, A. Markopoulos, O. Meca, O. Vysocký, T. Kozubek, V. Vondrák. A massively Parallel and Memory Efficient FEM Toolbox with a Hybrid Total FETI Solver with Accelerator Support. *The International Journal of High Performance Computing Applications*. 2018. DOI: 10.1177/1094342018798452. Q2, IF=2,015.

The Parallel Algorithms Research Lab cooperates, for example, with an engineering company in pump efficiency optimization using an open source solution and HPC



Advanced Data Analysis and Simulations Lab

Significant events

- > Successful submission of the international H2020 **LEXIS** (Large-scale EXecution for Industry & Society) project in the domain “ICT-11-2018-2019: HPC and Big Data enabled Large-scale Test-beds and Applications”. The project was approved for funding at the beginning of January 2019. IT4Innovations is the coordinator of the project, which involves 15 other international partners.
- > Two outputs of the laboratory were nominated for the **European Commission's Innovation Radar Prize**. The **Hyperloom** application for easy processing of data using supercomputers was nominated in the Excellent Research category, and the **Intelligent online navigation system for citizens** developed in cooperation with Sygic was nominated in the Early Stage Innovation category. The intelligent navigation advanced to the final based on voting.
- > Successful defence and completion of the **ESA TEP URBAN Turbo-Hub** project. At the end of the project, more than 330 institutions from more than 40 countries applied for access to the products and services provided by the developed Urban TEP platform. Continuation of the activities is ensured in the follow-up **ESA URBAN TEP II** project having already been taking place since 2018 with the objective to develop a self-sufficient and sustainable platform for urban satellite images analysis.

- > The **ExCAPE** project was successfully defended and completed. The project included development of the HyperLoom platform, which was fully used in experiments within the project. The platform is being further modified to be used in the ExaQute project.
- > Georg Zitzlsberger received an **NVIDIA Deep Learning Institute (DLI) instructor certificate**. As the NVIDIA DLI Ambassador for VSB – Technical University of Ostrava, he will lead the Fundamentals of Deep Learning for Computer Vision course in 2019.
- > Tomáš Martinovič defended his dissertation “Tools for Time Series Analysis of Nonlinear Dynamical Systems” in the field of Computational sciences in December 2018 under the supervision of Doc. Marek Lampart. The work received the Best Dissertation Award 2018 in the Information technology category in the international competition announced by the PROGRES 3 university consortium.

Selected publications

- > Ovečka, M., D. von Wangenheim, P. Tomančák, O. Šamajová, G. Komis, J. Šamaj. Multiscale Imaging of Plant Development by Light-sheet Fluorescence Microscopy. *Nature Plants*. 2018, 4(9), 639–650. DOI: 10.1038/s41477-018-0238-2. Q1, IF=11,471.

- > Ruiz-Constán, A., A. M. Ruiz-Armenteros, S. Martos-Rosillo, J. Galindo-Zaldívar, M. Lazecký, et al. SAR Interferometry Monitoring of Subsidence in a Detritic Basin Related to Water Depletion in the Underlying Confined Carbonate Aquifer (Torremolinos, southern Spain). *Science of the Total Environment*. 2018, 636, 670–687. DOI: 10.1016/j.scitotenv.2018.04.280. Q1, IF=4,61.
- > Praks, P., and D. Brkić. One-log Call Iterative Solution of the Colebrook Equation for Flow Friction Based on Padé Polynomials. *Energies*. 2018, 11(7). DOI: 10.3390/en11071825. Q2, IF=2,676.
- > Lampart, M., J. Zapoměl. The Motion Characteristics of the Double-pendulum System with Skew Walls. *Mathematical Methods in the Applied Sciences*. 2019; 42(2), 475–487. DOI: 10.1002/mma.5354. Q2, IF=1,18.
- > Lampart, M., J. Zapoměl. Mathematical Methods in the Applied Sciences. 2018, 41(17), 7106–7114. DOI: 10.1002/mma.4650. Q2, IF=1,18.



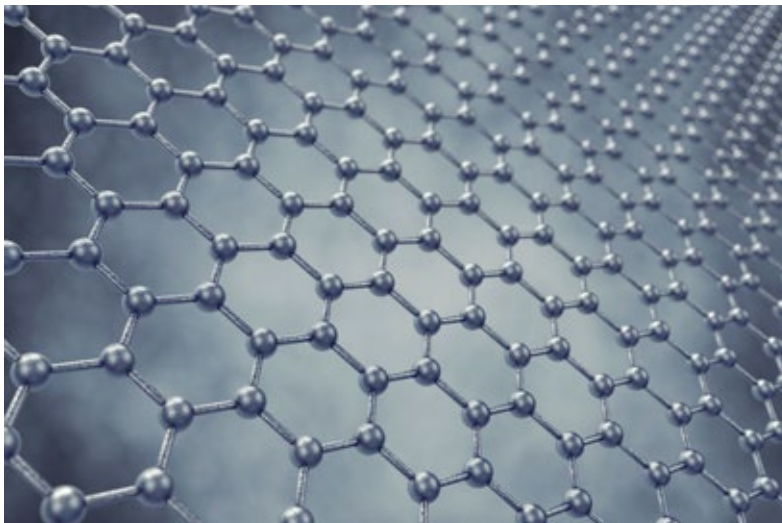
The Advanced Data Analysis and Simulations Lab provides, for example, HPC as a Service for hydrologic modelling

Significant events

- > Tibor Fördös successfully defended his **dissertation** before the French-Czech committee in Paris (at l'Ecole Polytechnique, Palaiseau) in July 2018.
- > Participation at the 2nd **French-Czech Barrande Workshop**, which was held in Paris in October in 2018.

Selected publications

- > Zhang, S., D. Legut, Z. Fu, T. C. Germann, and R. Zhang. High-throughput Screening for Superhard Carbon and Boron Nitride Allotropes with Superior Stiffness and Strength. Carbon. 2018, 137, 156-164. DOI: 10.1016/j.carbon.2018.05.020. Q1, IF=7,082.
- > Halagačka, L., M. Vanwolleghem, F. Vaurette, J. B. Youssef, K. Postava, J. Pištora, and B. Dagens. Magnetoplasmonic Nanograting Geometry Enables Optical Nonreciprocity Sign Control. Optics Express. 2018, 26(24). DOI: 10.1364/OE.26.031554. Q1, IF=3,356.
- > Fördös, T., K. Postava, H. Jaffrès, D. Quang To, J. Pištora, and H. J. Drouhin. Mueller Matrix Ellipsometric Study of Multilayer Spin-VCSEL Structures with Local Optical Anisotropy. Applied Physics Letters. 2018, 112(22). DOI: 10.1063/1.5009411. Q1, IF=3,495.
- > Mrázková, Z., I. P. Sobkowicz, M. Foldyna, K. Postava, I. Florea, J. Pištora, and P. Roca i Cabarrocas. Optical Properties and Performance of Pyramidal Texture Silicon Heterojunction Solar Cells: Key Role of Vertex Angles. Progress in Photovoltaics: Research and Applications. 2018, 26(6), 369-376. DOI: 10.1002/pip.2994. Q1, IF=6,456.
- > Mičica, M., S. Eliet, M. Vanwolleghem, et al. High-Resolution THz Gain Measurements in Optically Pumped Ammonia. Optics Express. 2018, 26(16). DOI: 10.1364/OE.26.021242. Q1, IF=3,356.



The Modelling for Nanotechnologies Lab is focused on development of novel materials and the study of their surface magneto-optical properties

Big Data Analysis Lab

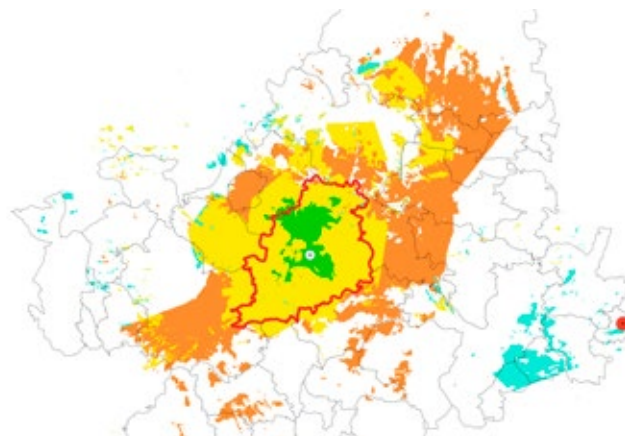
Significant events

- > Funding approved for the new H2020 **“Open European Quantum Key Distribution Testbed”** (OPENQKD) project in the field of cybernetic security within the SU-ICT-04-2019 call. The project is coordinated by the Austrian Institute of Technology and is focused on highly secured networks using the components of quantum mechanics for quantum key distribution. The overall budget of the project consortium amounts to EUR 15 million, thus making the project one of the key security plans in terms of the volume of funding that the European Commission has ever supported.

The issue of localization accuracy and localization error demonstrated for a randomly selected municipality. The image illustrates technical and spatial conditions, which need to be taken into account when relating the observation of the phenomenon occurring in the functional division to the administrative division. White dot – geometric centre of the observed municipal administrative division, red bounded polygon – the borders of the municipal administrative area, transparent polygons – the borders of the administrative area of municipalities covered with same cells, red dot - the most distant inhabited place, colourful polygons – mobile network coverage.

Selected publications

- > Továrek, J., G. H. Ilk, P. Partila, and M. Vozňák. Human Abnormal Behavior Impact on Speaker Verification Systems. IEEE Access. 2018, 6, 40120–40127. DOI: 10.1109/ACCESS.2018.2854960. Q1, IF=3,557.
- > Nguyen, T. N., T. H. Quang Minh, P. T. Tran, M. Vozňák, T. T. Duy, T.-L. Nguyen, and P. T. Tin. Performance Enhancement for Energy Harvesting Based Two-Way Relay Protocols in Wireless Ad-hoc Networks with Partial and Full Relay Selection Methods. Ad Hoc Networks. 2019, 84, 178–187. DOI: 10.1016/j.adhoc.2018.10.005. Q1, IF=3,151.
- > Nguyen, T. N., P. T. Tin, D. H. Ha, M. Vozňák, P. T. Tran, M. Tran, and T.-L. Nguyen Hybrid TSR–PSR Alternate Energy Harvesting Relay Network over Rician Fading Channels: Outage Probability and SER Analysis. Sensors. 2018, 18(11). DOI: 10.3390/s18113839. Q2, IF=2,475.
- > Nguyen, T. N., M. Tran, P. T. Tran, P. T. Tin, T.-L. Nguyen, D.-H. Ha, and M. Vozňák. On the Performance of Power Splitting Energy Harvested Wireless Full-Duplex Relaying Network with Imperfect CSI over Dissimilar Channels. Security and Communication Networks. 2018, 1–11. DOI: 10.1155/2018/6036087. Q4, IF=0,904.
- > Eglynas, T., M. Jusic, S. Jakovlev, A. Senulis, A. Andziulis, S. Gudas. Analysis of the Efficiency of Shipping Containers Handling/Loading Control Methods and Procedures. Advances in Mechanical Engineering. 2019, 11(1). DOI: 10.1177/1687814018821229. Q4, IF=0,848.



Significant events

- > Awarded the Best Poster Award for the paper titled “Workflow for Parallel Processing of Sequential Mesh Databases” at the Supercomputing Conference, November 2018, Dallas, USA.
- > The promotional movie Agent 327: Operation Barber Shop, rendered using the IT4Innovations infrastructure in cooperation with the Blender Institute, won the prestigious global Webby Awards.
- > Successful defence and completion of the READEX project funded by the European Union Framework H2020 programme.
www.readex.eu
- > As a follow-up of the Performance Optimisation and Productivity 1 (POP1) project, the POP2 HPC Centre of Excellence project was awarded funding to focus on optimization of parallel applications running on HPC infrastructure.
www.pop-coe.eu
- > Cooperation within the READEX project led to the publishing of a chapter in the System Scenario-based Design Principles and Applications publication: Kjeldsberg, P.G., R. Schone, M. Gerndt, L. Říha, V. Kannan, K. Diethelm, M-C. Sawley, J. Zapletal, O. Vysocký, M. Kumaraswamy, and W. E. Nagel. Runtime Exploitation of Application Dynamism for Energy-efficient Exascale Computing, Springer International Publishing AG. It is to be published in 2019.
- > Jan Zapletal, an IT4Innovations researcher and graduate of the Faculty of Electrical Engineering and Computer Science, VSB – Technical University of Ostrava, won 1st place in the Competition for the Best Dissertation titled “The Boundary Element Method for Shape Optimization in 3D” and defended in 2017. The prize was awarded in the Information technology and Electrical engineering category by VSB-TUO and the Progres 3 consortium.
- > Jan Zapletal has moved on to the finals in the national competition for the Antonín Svoboda Award, announced by the Czech Society for Cybernetics and Informatics.



Selected publications

- > Malý, L., J. Zapletal, M. Merta, L. Říha, and V. Vondrák. Evaluation of the Intel Xeon Phi Offload Runtimes for Domain Decomposition Solvers. *Advances in Engineering Software*. 2018, 125, 146-154. DOI: 10.1016/j.advengsoft.2018.06.011. Q1, IF=3,198.
- > Zapletal, J., G. Of, and M. Merta. Parallel and Vectorized Implementation of Analytic Evaluation of Boundary Integral Operators. *Engineering Analysis with Boundary Elements*. 2018, 96, 194-208. DOI: 10.1016/j.enganabound.2018.08.015. Q2, IF=2,138.
- > Říha, L., M. Merta, R. Vavřík, T. Brzobohatý, A. Markopoulos, O. Meca, O. Vysocký, T. Kozubek, and V. Vondrák. A Massively Parallel and Memory-Efficient FEM Toolbox with a Hybrid Total FETI Solver With Accelerator Support. *The International Journal of High Performance Computing Applications*. 2018. DOI: 10.1177/1094342018798452. Q2, IF=2,015.
- > Dohr, S., J. Zapletal, G. Of, M. Merta, and M. Kravčenko. A Parallel Space-Time Boundary Element Method for the Heat Equation. *Computers & Mathematics with Applications*. DOI: 10.1016/j.camwa.2018.12.031. Q1, IF=1,860.
- > Scionti, A., S. Mazumdar, and A. Portero. Towards a Scalable Software Defined Network-on-Chip for Next Generation Cloud. *Sensors*. 2018, 18, 2330. DOI: 10.3390/s18072330. Q2, IF=2,475.
- > Kumaraswamy, M., A. Chowdhury, M. Gerndt, Z. Bendifallah, O. Bouizi, L. Říha, O. Vysocký, M. Beseda, and J. Zapletal. Domain Knowledge Specification for Energy Tuning. *Concurrency and Computation: Practice and Experience*. 2018. DOI: 10.1002/cpe.4650. Q3, IF=1,114.

CC-BY, Blender Institute, image from The Daily Dweebs – demonstration of the model and final visualization. IT4Innovations cooperates with the Blender Institute in visualizations of computer-generated scenes. We are developing CyclesPhi, a module allowing the use of the computing capacity of the whole supercomputer, including its acceleration cards of the Intel Xeon Phi type for rendering.



National Grants

IT4Innovations Excellence in Science (2016–2020)

PROJECT ID LQ1602

PRINCIPAL INVESTIGATOR

Prof. Tomáš Kozubek

In the years 2011 to 2015, the IT4Innovations Centre of Excellence project was jointly implemented by the following partners: VSB – 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 Dominik Legut

The project aims to investigate the characteristics of the selected two-dimensional magnetically-frustrated quantum system $\text{Cu}(\text{tn})\text{Cl}$ ($\text{tn}=1.3$ -diaminopropan = $\text{C}_3\text{H}_{10}\text{N}_2$) 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.

NEW

Understanding of the Magnetostriction in Fe-Ti Alloys by First-principles Calculations (2018–2019)

PROJECT ID 8J18AT004

PRINCIPAL INVESTIGATOR

Dr Dominik Legut

This project is focused on a theoretical identification of mechanisms that control the reduction and/or suppression of the thermal expansion of the dual-phase magnetostrictive Ti-based alloys. Concepts for controlling the thermal expansion may make use of a mixture of two phases, doping by an sp-element or using anti-ferromagnetic ordering in one of the phases in selected transition-metal (TM)-Ti alloys.

NEW

Metal-graphene Interfaces – Foundations of Novel Spintronic Materials (2018–2019)

PROJECT ID 8J18DE004

PRINCIPAL INVESTIGATOR

Dr Dominik Legut

The main objective of this study is the investigation of magnetization effects in graphene induced by magnetic layers like Co, Ni, Fe-alloys, e.g. FeCo. The applied spectroscopy is reflection polarization spectroscopy and total electron yield (absorption) spectroscopy with soft x-ray synchrotron radiation across the carbon 1s resonance energy. This advance topic follows the basic optical characterization (optical constants) by means of the theoretically calculated

and experimentally measured magneto-optical effects of graphene and highly oriented pyrolytic graphite (HOPG) on various magnetic and nonmagnetic substrates.

NEW

Modeling of Interactions of Cold Rare-gas Plasmas with Ambient Air (2018–2019)

PROJECT ID 8J18FR031

PRINCIPAL INVESTIGATOR

Doc. René Kalus

The project aims at performing extensive ab initio calculations to deeply understand the interactions in $[\text{He}/\text{X}_2]^+$ ($\text{X} = \text{N}, \text{O}$) collision systems including excited electronic states and transitions between them. Another objective is to create a suite of codes for non-adiabatic dynamics simulations linking hybrid dynamical approaches with on-the-fly ab initio calculations. Using the codes created within the project, pilot dynamical calculations on a selected collision systems, He^+/X_2 ($\text{X} = \text{N}, \text{O}$) will be performed, with the main aim to get collision cross-sections to be further used in macroscopic modelings. The collision cross-sections will be used in calculations of transport properties (mobilities) of He^+ ions in X_2 ($\text{X} = \text{N}, \text{O}$). The reliability of the theoretical approaches will be compared against experimental data.

GRANTS OF MEYS FOR SPECIFIC UNIVERSITY RESEARCH FOR THE YEAR 2018

Optimization of Machine- learning Algorithms for an HPC Platform II

PROJECT ID SP2018/142

PRINCIPAL INVESTIGATOR

Martin Golasowski

The project was focused on the use of algorithms of unsupervised machine learning for preprocessing the data for supervised machine learning algorithms. The objective of this project was to link a suitable algorithms developer in the 1st phase of the project and to perform implementation for an HPC platform focused on real large datasets and their continuous processing.

Dynamic Systems Problems and their Implementation on HPC

PROJECT ID SP2018/173

PRINCIPAL INVESTIGATOR

Dr Tomáš Martinovič

The objective of the project was to design and implement parallel algorithms for solving dynamic systems problems. Special attention was paid to methods for nonlinear dynamic systems analysis, the chaos theory, and operations research. In implementation of this project, knowledge acquired from the previous SGS 2017/182 project was applied.

Hardware Acceleration of Matrix Assembler and GUI Development of ESPRESO Library

PROJECT ID SP2018/159

PRINCIPAL INVESTIGATOR

Radim Vavřík

The project aimed at optimizing a part of the FEM based ESPRESO library code for x86 architectures (primarily Intel Xeon or Intel Xeon Phi Knights Landing) and GPU accelerators supporting the CUDA technology. Other parts of the project included development of a graphical user interface (GUI) for the configuration of problems solved using the ESPRESO library. The project output was an improved ESPRESO code of higher performance in solving real engineering problems, and its extension with the GUI module.

Development of Tools for HPC Applications Energy Optimization

PROJECT ID SP2018/134

PRINCIPAL INVESTIGATOR

Ondřej Vysocký

The contribution of the proposed project was extension of MERIC, a tool for supporting new architectures (Intel Xeon Phi, ARM, and others) allowing their evaluation in terms of their energy consumption and potential savings when static and dynamic tuning of SW as well as HW parameters is performed. The RADAR tool was extended with a graphical user interface and other methods for evaluation of measured data.

Solving Problems with Uncertainties Using the Boundary Element Method

PROJECT ID SP2018/161

PRINCIPAL INVESTIGATOR

Michal Běreš

The project built on the previous SGS SP2017/165, SGS SP2016/113, and SP2015/160 projects, and its objective was to use BEM4I, an existing library of parallel boundary element-based solvers, to solve problems with uncertainties. The project was mainly focused on the use of the BEM4I library as an efficient “black-box” solver for problems dealing with propagation of uncertainties from input parameters and for solution of inversion uncertainty problems in measurement.

Internationalization of Doctoral Education in Molecular Physics

PROJECT ID SP2018/178

PRINCIPAL INVESTIGATOR

Martin Mrovec

The principal objective of the project was to further develop the internationalization of the MOLDYN group in scientific education of postgraduate students. Particularly, it included building on the cooperation established within the internships done abroad in 2017. The cooperation took place at the research workplaces at UPS in Toulouse (low-temperature plasma modelling for biomedical applications and mathematical modelling of molecular interactions) and at UPEM in Paris (quantum Monte Carlo methods).

Application of Topology Optimization Methods in Engineering Practice

PROJECT ID SP2018/180

PRINCIPAL INVESTIGATOR

Dr Pavel Maršálek

The contribution of the project was to expand knowledge within IT4Innovations with a new application area of significant commercial potential. Within the project, the investigators became familiar with topology optimization from both the theoretical and practical point of view, learning about the methods of topology optimization and particular real engineering problems, respectively.

Hydroxyapatite Nanocomposites: Structure and Modelling

PROJECT ID SP2018/166

PRINCIPAL INVESTIGATOR

Lenka Pazourková

The project was aimed at preparing and characterizing calcium phosphates – Ca-deficient hydroxyapatite (CDH)- and clay materials-based nanocomposites. Within molecular modelling, analysis of Ca-deficient hydroxyapatite composite interaction was performed by means of molecular dynamics using empirical force fields.

Modelling of Diffractive and Plasmonic Nanostructures

PROJECT ID SP2018/83

PRINCIPAL INVESTIGATOR

Tomáš Kohut

The objective of this project was to study and model polarimetric responses from holographic structures using the Kirchhoff scalar integral and Stratton-Chu-Silver vector integral in a Mueller matrix form. The project also aimed at modelling of metamaterial plasmonic surface using the boundary element method in order to change wave phase, thus create a holographic image.

Ellipsometry and Magneto-optical Properties of Pr and Nd Based Perovskites and MO Effect in Cubic (011) Oriented Transition Metals Layers on MgO Substrate

PROJECT ID SP2018/96

PRINCIPAL INVESTIGATOR

Radek Ješko

The focus of this project was on two main research areas. In cooperation with the Faculty of Mathematics and Physics of Charles University in Prague, spectroscopic ellipsometric and magneto-optic measurements of volume samples of orthorhombic oxides were performed. Quadratic magneto-optic spectra (QMOKE) of cubic structures with (011) oriented surface, in particular thin layers of iron and cobalt on MgO substrate, were also measured.

Project supported by the Grant Agency of the Czech Republic

Novel Fuel Materials for Generation IV Nuclear Reactors

PROJECT ID GA17-27790S

PRINCIPAL INVESTIGATOR

Dr 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 the thermal expansion of actinide carbides, and especially the negative thermal expansion observed in UC2 at the atomic level.

Projects supported by the Technology Agency of the Czech Republic

Centre of Competence for Molecular Diagnostics and Personalized Medicine (2014–2019)

PROJECT ID TE02000058

(project supported by the Centre of Competence programme)

PRINCIPAL INVESTIGATOR

Dr Branislav Janský

The primary objective of the project is to apply and further foster the existing expert experience and to achieve a critical mass of participants and knowledge in research, development, manufacturing, protection of Intellectual Property, certification, technology transfer, and commercialization 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)

PRINCIPAL INVESTIGATOR

Dr 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.

Projects of Operational Programme Research, Development and Education

IT4Innovations National Supercomputing Center – Path to Exascale (2017–2021)

PROJECT ID EF16_013/0001791

PRINCIPAL INVESTIGATOR

Dr Branislav Janský

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 the services provided by this infrastructure to its users.

Artificial Intelligence and Reasoning (2017–2022)

PROJECT ID

CZ.02.1.01/0.0/0.0/15_003/0000466

PRINCIPAL INVESTIGATOR

Prof. Václav Snášel

The AI and Reasoning project yields significant measures for the development of informatics, robotics, and cybernetics research at the Czech Technical University in Prague. The project envisions the establishment of a new AI and

Reasoning research group within a given part of the Czech Institute of Informatics, Robotics, and Cybernetics (CIIRC), which focuses on solving advanced interdisciplinary problems of high technical as well as social priority. The project is also supported by national partners (VSB – Technical University of Ostrava and the University of West Bohemia in Pilsen). The motivation for their participation is based on the emphasis on concentration and integration of resources, sharing of knowledge and infrastructure, and last but not least, on establishing a “unified space for opportunities” for young talent in the Czech Republic.

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 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. Managing their runtime and implementation of auto-tuning will enable us to achieve energy-efficient heterogeneous HPC systems on the exascale level.

www.antarex-project.eu

Projekty

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

PROJECT ID 671555

(H2020-FETHPC-2014 call)

PRINCIPAL INVESTIGATOR

Dr Jan Martinovič

Within this project, IT4Innovations was involved in development of state-of-the-art scalable algorithms and their implementations suitable for running on future Exascale machines. The relevant algorithms were developed for solving complex problems in the field of pharmacology, with respect to the necessity of processing large data sets, which is 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 Lubomír Říha

The role of IT4Innovations in this project was the 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 Environmental Impact Brake System (2015–2019)

PROJECT ID 636592

(H2020-MG-2014_TwoStages call)

PRINCIPAL INVESTIGATOR

Prof. 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. Tomáš Kozubek

The objective of this four-year long project is to educate researchers able to participate in interdisciplinary co-operation. 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

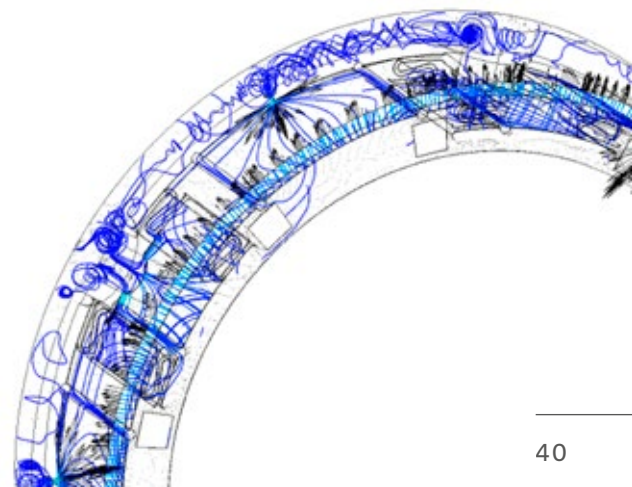
(H2020-ICT-2016-2 call)

PRINCIPAL INVESTIGATOR

Karina Pešatová, MBA

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 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 project aims at optimization of production processes and productivity of companies using HPC-based modelling and simulation as well as cloud services.

www.cloudifacturing.eu

NEW

ExaQute – Exascale Quantifications of Uncertainties for Technology and Science Simulation (2018–2021)

PROJECT ID 800898

(H2020-FETHPC-2016-2017)

PRINCIPAL INVESTIGATOR

Dr Tomáš Karásek, and Dr Jan Martinovič

The objective of ExaQute, a three-year project, is to develop new methods allowing solution of complex engineer-

ing problems using numerical simulations on future exascale systems. Within the project, new computing methods and software tools will be developed for solving simulations of aerodynamics for optimizing geometrically complex civil engineering structures. IT4Innovations will participate in deploying the Hyperloom and COMPSs tools using high performance computing systems, their configuration, and optimization. Our participation also includes testing of robust algorithms for shape optimization of wind-loaded structures.

www.exaqute.eu

NEW

POP2 - Performance Optimisation and Productivity 2 (2018–2021)

PROJECT ID 824080

(H2020-INFRAEDI-2018-1)

PRINCIPAL INVESTIGATOR

Dr Lubomír Říha

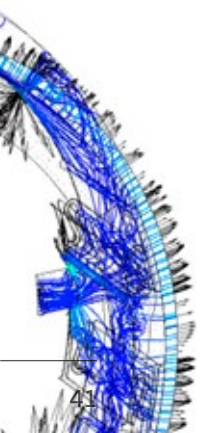
The POP2 Centre of Excellence in HPC builds on the Performance Optimisation and Productivity 1 (POP1) project and extends its activities. The main aim of POP2 is to assist with analysis of parallel applications, identification of erroneous parts of codes, and recommendations of optimization methods resulting in increased performance and better scalability of a given application.

<https://pop-coe.eu/>

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 2018 included collaboration with 17 companies:

- > AL INVEST BŘIDLIČNÁ a.s.
- > BANK FOR INTERNATIONAL SE
- > BAYNCORE LIMITED
- > BORCAD cz s.r.o.
- > Continental Automotive Czech Republic s.r.o.
- > Doosan Škoda Power s.r.o.
- > ING corporation, spol. s.r.o.
- > INSET s.r.o.
- > Invent Medical Group s.r.o.
- > IXPERTA s.r.o.
- > K2 atmitec s.r.o.
- > KOMA – Industry s.r.o.
- > mySASY a.s.
- > Siemens s.r.o.
- > Strojírny a stavby Třinec a.s.
- > The German Aerospace Center
- > Forest Management Institute



EDUCATIONAL AND TRAINING ACTIVITIES

PhD Study Programme

The Computational Sciences PhD study programme was opened at IT4Innovations in the academic year 2015-2016. Students are focused on the use of HPC and HPDA in science and industry. In December 2018, two students successfully completed their studies within this programme. A total of 21 students participated in the study programme as of the end of the year 2018.

Educational Activities

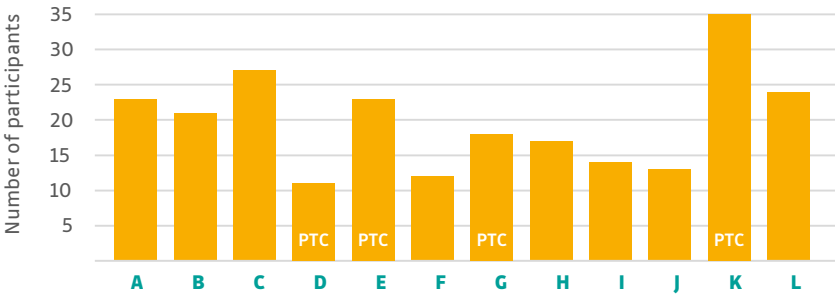
IT4Innovations supports the scientific community as well as its users by organizing high-quality courses, tutorials, workshops, and other educational events. The primary objective of these activities is to broadly enhance competencies of users in terms of efficient use of the unique IT4Innovations supercomputing infrastructure. In a broader sense, IT4Innovations aims at increasing awareness and knowledge of the field of HPC nationwide among interested members of both academia and industry.

The topics of courses offered by IT4Innovations are focused on computer systems and architectures, programming techniques and tools, and libraries and applications.

In 2018, a total of 12 educational events attended by almost 240 participants were held. The most important ones led by renowned foreign experts were as follows:

- > **HIGH PERFORMANCE DISTRIBUTED DEEP LEARNING** (Dhabaleswar K. Panda, Hari Subramoni, Ammar Ahmad Awanz from the Ohio State University), which presented the effect of advanced optimizations and tuning of libraries using CUDA-Aware MPI on performance of deep neural networks training;

Educational activities in 2018



- A** InfiniBand, Omni-Path and High-Speed Ethernet for Dummies

B InfiniBand, Omni-Path and High-Speed Ethernet: Advanced Feature, Challenges in Designing, HEC Systems and Usage

C High Performance Distributed Deep Learning

D Intel Xeon Phi Programming

E Parallel I/O and Libraries
- F** Current GPU Programming Trends

G PETSc Basic and Advanced Tutorial

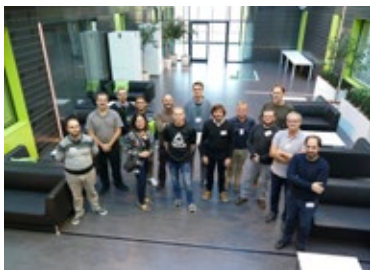
H HyperLoom

I PLASMA and MAGMA

J ANTAREX

K Productivity Tools for HPC

L Advanced OpenMP Programming



- > **INFINIBAND, OMNI-PATH, AND HIGH-SPEED ETHERNET: ADVANCED FEATURES, CHALLENGES IN DESIGNING, HEC SYSTEMS AND USAGE TUTORIAL** (Dhabaleswar K. Panda, Hari Subramoni, Ammar Ahmad Awanz from the Ohio State University) focused on advanced hardware and software functions of technologies such as InfiniBand, Omni-Path, High-speed Ethernet as well as RDMA over Converged Enhanced Ethernet; the course included Open Fabrics RDMA and Libfabrics programming or infrastructure for administration and tools for efficient use of these connecting systems;
- > two-day **ADVANCED OPENMP PROGRAMMING - HOST PERFORMANCE AND ACCELERATOR OFFLOADING COURSE** (Christian Terboven, Tim Cramer), which presented the OpenMP parallelization method and its new functions for the best possible use on modern computer architectures.

In 2017, IT4Innovations received the status of PRACE Training Center (PTC) and in 2018 organized four courses. The most successful course in terms of the number of participants was Productivity Tools for High Performance Computing led by the IT4Innovations employees (Branislav Jansík, David Hrbáč, Josef Hrabal, Lukáš Krupčík, Lubomír Prda, and Roman Slíva). The objective of the course was to develop the skills and increase the knowledge of the participants in managing the tools and technologies used in the IT4Innovations clusters.

It included, for example, GIT, KVM, Docker&Singularity, and EasyBuild. Another PTC course organized was, for example, Parallel I/O and Libraries (Nicole Audiffren z CINES, France, Sebastian Lührs from JSC, Germany), which presented MPI-IO and HDF5 and SIONlib libraries.

Award of NVIDIA Deep Learning Institute certification

Thanks to Georg Zitzlsberger, IT4Innovations has become an NVIDIA Deep Learning Institute Ambassador for universities. Mr Zitzlsberger was awarded the Fundamentals of Deep Learning for Computer Vision Instructor certificate at the end of the year 2018. This first successfully received certification provides a stepping stone for IT4Innovations to maintain long-term cooperation with the NVIDIA company. From the year 2019, IT4Innovations will offer practical courses to developers and researchers who would like to solve complex problems using deep learning.



PRACE Summer of HPC

Already for the sixth time, the Summer of HPC programme has offered students of European universities summer internships focused on HPC in the countries participating in the Partnership for Advanced Computing in Europe (PRACE) project. This summer, 23 students were given the opportunity to participate in summer internships at 11 host organizations. Two of these students were welcomed at IT4Innovations. One of them was James Lowe, a graduate of the Electronics and Communication bachelor study program at the Dublin Institute of Technology School of Electrical and Electronic Engineering, who worked on the High-level Visualizations of Performance Data project. Vladimir Nikolic, a student of Software engineering at the University of Belgrade, was involved in the Improving Existing Genomic Tools for HPC Infrastructure project.

Projects of Operational Programme Research, Development, and Education

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

Doc. René Kalus

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, the Czech Academy of Sciences, and VSB-TUO. Part of the project is to modernize and internationalize one of the doctoral programs of the school (Computational Sciences, VSB-TUO) as well as to create new double-degree programmes (planned in collaboration with Università della Svizzera italiana, Lugano, Switzerland, and l'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

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 m². 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.

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. René Kalus

The project of VSB – 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.

NEW

Science without Borders (2018–2020)

PROJECT ID CZ.02.2.69/0.0/0.0/16_027/0008463 (02_16_027 call)

IT4INNOVATIONS PROJECT

COORDINATOR: Prof. Tomáš Kozubek

The objective of the VSB – Technical University of Ostrava project is to implement 43 international mobilities,

which will lead to professional development, enhancement of qualification and other skills of both junior and senior researchers, thereby acquiring and transferring of experience abroad as well as ensuring foreign experts at VSB – Technical University of Ostrava. Mobilities shall allow participation in international chains of scientific laboratories and academic institutions primarily, although not exclusively, within the European Research Area (ERA), an increase in the intensity of establishing international contacts, and involvement in international R&D initiatives and projects.

International Visegrad Fund project

NEW

**Superheroes 4 Science
(2018–2020)**

PROJECT ID 21820033

PRINCIPAL INVESTIGATOR

Karina Pešatová, MBA

A joint project of partners from the Visegrad Four (IT4Innovations National Supercomputing Center, the Governmental Information Technology Development Agency of Hungary, the Computing Center of the Centre of Operations of the Slovak Academy of Sciences, Poznań Supercomputing and Networking Center – the Institute of Bioorganic Chemistry of the Polish Academy of Sciences) aims at

explaining attractively the importance of supercomputers and their use, which has a positive impact on the everyday life of people. Each project partner provides information about their national supercomputing infrastructure and dedicates substantial effort to popularisation activities focused on increasing awareness of supercomputing, its ever-increasing importance for society, and justification of investments therein. The understanding of both scientific topics and super-

computing is not easy for non-experts at all. In order to make communication of the relatively complex content easier, the resulting materials will be adapted to different target groups based on the age, level of education as well as qualification. The objective of the project is to not only educate the wider public, but to also inspire the younger generation in Visegrad countries to enrol for scientifically and technologically oriented study programmes.



*Illustration
from the
Designer's
Nightmare
comic
created
within the
Superheroes
4 Science
project*



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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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