REVIEW 2020

Our supercomputers support science, industry, and society.

MANAGING DIRECTOR'S INTRODUCTION

Dear readers,

Let me begin by summarizing, as I do every year, what has been going on in our supercomputing centre during the past year. This past year has been significantly different from previous ones. The COVID-19 pandemic touched everyone's life, and so did the activities of our centre. We have experienced the advantages and disadvantages of home office, which, although it brings with it greater flexibility, often makes the process of implementing the activities we have committed to lengthier and more complicated. Even though time almost stopped for the company for a while, it did not derail our activities, and we accomplished a lot in the past year.

In 2019, we succeeded in a pan-European competition with the „IT4Innovations Centre for European Science and Industry" project to host one of the EuroHPC petascale supercomputing systems to be built within the EuroHPC Joint Undertaking. A public procurement procedure for the supplier of this system was undertaken last year, which resulted in the signing of a contract between IT4Innovations, EuroHPC JU, and Hewlett Packard Enterprise as the supplier of the system. A public competition for the name of this new supercomputer was also held. The name Karolina will follow the precedent of previous supercomputers being named after historically and regionally significant figures. Karolina will bring a peak performance of 15.7 PFlop/s to its users and will serve not only the Czech but also European scientific communities and industrial partners.

However, the other supercomputers of our centre were not left behind either, as with their help we actively participated in several projects in the fight against COVID-19. Immediately after the outbreak of the pandemic in the Czech Republic, we responded to the situation and offered our users priority access to computational resources for solving research problems related to COVID-19. Another important project, for which the Big Data Analysis lab is responsible, is the Mobility Atlas. This is the primary data interface providing information about the mobility of people in the Czech Republic during the state of emergency, processed from anonymized T-Mobile CZ traffic data on our supercomputers. Last but not least, as the only Czech representative in the prestigious Exscalate4COV project supported by the European Commission, we have been actively involved in research activities in the search for coronavirus drug treatments.

However, our supercomputers also provided their computing power to address research goals of our users that are not related to the COVID-19 pandemic. Among their projects solved using our supercomputers, I would like to highlight the project of Pavel Jungwirth and his research team from the Institute of Organic Chemistry and Biochemistry of the CAS, which answers the question of what metal is and how it is actually formed. The result of this project even made the cover of one of the most prestigious and most cited scientific journals in the world: Science.

Our research activities have not stopped either. In particular, I would like to mention the acquisition and start of new Horizon 2020 as well as EuroHPC projects. Since last year, we have been the National Competence Centre in HPC within the EuroCC project, which is the reference and single point of contact and coordination in the Czech Republic for high-performance computing and data analysis. Within the evaluation of our research activities by an international evaluation panel according to Module 3 of the RIV 2017+ methodology, IT4Innovations received the highest grade of 5: Excellent.

It is also important to recognize our cooperation with industrial companies, which is an integral part of our activities, and which we continually seek to expand. The Digital Innovation Hub Ostrava, which we have established together with the Moravian-Silesian Innovation Centre, should help us significantly in this area. Together, we will try to help companies, especially from the Moravian-Silesian Region, to address their needs in the field of digitalisation. Thanks to our research and innovation activities, the Moravian-Silesian Region, the City of Ostrava, and the entire Czech Republic have been listed among the top IT centres in Europe. The recently published Innovation Radar on the European Commission's website makes IT4Innovations and our region clearly visible on the map of Europe.

Unfortunately, not only pleasant events befell us. Last year, we bid farewell to our long-time colleague, Professor Jaromír Pištora, who successfully led the Modelling for Nanotechnologies Lab for many years, and was behind the foundation of IT4Innovations at the very beginning. Let me at least take this opportunity to thank him for his contribution in the development of our centre.

Finally, I would also like to thank all our employees and partners who, in difficult times, have continuously contributed to the fulfilment of our strategic goals and commitments, ensuring the operation of our centre and contributing to its further development. I hope that in the years to come we will not have to face the obstacles that befell us last year.

Vít Vondrák

IT4Innovations National
Supercomputing Center

IMPORTANT EVENTS IN 2020
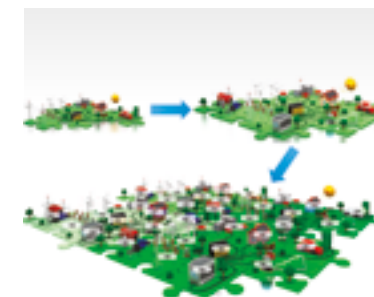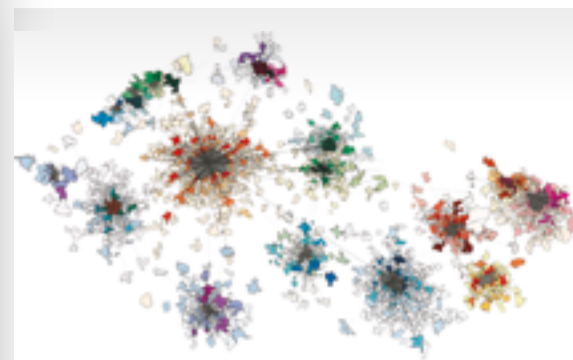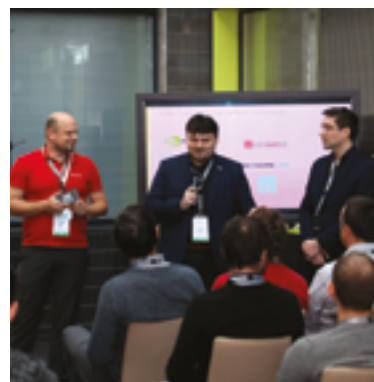
JANUARY

> IT4Innovations and the Moravian-Silesian Innovation Centre Ostrava concluded a memorandum establishing the **Digital Innovation Hub Ostrava**.

> Research activities within **the Research and Development of a Functional Sample of a Railway Vehicle Enabling Collection of Data and Software – a Simulator Enabling Generation of Data to Train Obstacle Detection under Simulated Conditions** project kicked off. It was supported in the 1st Open Call of the Technology Agency of the Czech Republic as part of the TREND programme for industrial research and experimental development.

> The launch of a project entitled **Blockchain ENabled DEep Learning for Space Data** (BLENDED), which was announced within the European Space Agency (ESA) Open Call.

FEBRUARY

> The **NVIDIA AI & HPC Academy 2020** was organised for all fans of artificial intelligence (AI) and high-performance computing (HPC) at IT4Innovations. It was a series of hands-on NVIDIA Deep Learning Institute workshops with 90 participants who learnt about optimal design and implementation of artificial intelligence algorithms on supercomputers.

> Georg Zitzlsberger was awarded two **certificates in the field of Deep Learning and AI**; Fundamentals of Deep Learning for Multiple Data Types and Fundamentals of Deep Learning for Multi-GPUs.

MARCH

> A modernised department for the research activities of the Modelling for Nanotechnologies Lab is equipped with a special **laser for the generation of ultrashort femto-second pulses**, i.e. laser beams with duration of a quadrillionth of a second (10-15 s).

APRIL

> IT4Innovations offers **priority use of computational resources** for projects related to COVID-19 disease mitigation.

> In cooperation with T-Mobile Czech Republic a. s., we cooperate in the extraction of anonymised population mobility data for the needs of the state to evaluate the impact of anti-epidemiological measures on population mobility; **the Mobility Atlas project**.

MAY

> The article titled **Domain Knowledge Specification for Energy Tuning**, which was co-authored by our colleagues Lubomír Říha, Ondřej Vysocký, Martin Beseda, and Jan Zapletal, is one of the 10% of the most downloaded contributions of the journal Concurrency and Computation: Practice and Experience.

> The strategic project titled **Smart Energy Grid Management System** (ES4G) started. The project brings together a unique research consortium; ENET and IT4Innovations at VSB-TUO, Brno University of Technology in Brno, and application sponsors E.ON Distribuce, a.s., ČEZ Distribuce, a. s., and ABB s.r.o.

JUNE

> We provide a service to our users to facilitate research and development within the international H2020-funded POP2 Centre of Excellence project. It offers **free assistance in optimization of parallel applications performance**.

> **New IT4Innovations website** launched. Not only the design of the website changed but also the content. The new website is fully responsive and available on all mobile devices.

> The scientific team from Pavel Jungwirth's group from the Institute of Organic Chemistry and Biochemistry (IOCB) of the CAS and their project made it onto the cover of one of the most prestigious and most cited scientific journals in the world: **Science.** IT4Innovations contributed to this discovery by allocating 650,000 core hours of computational resources to Pavel Jungwirth's research.

IMPORTANT EVENTS IN 2020
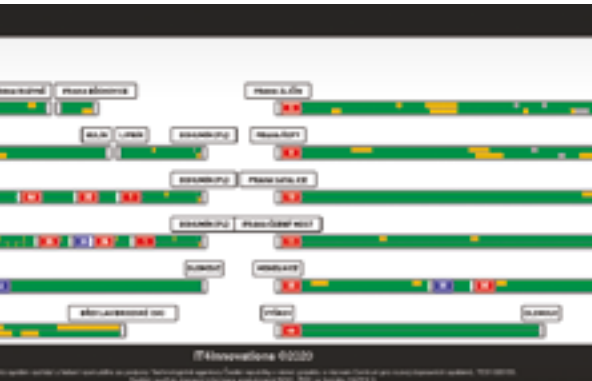
JULY

> IT4Innovations presents the **updated viaRODOS application**, which was developed within the RODOS project and is compatible with the Floreon+ system. The application uses data sources provided by the National Transport Information Centre (NDIC), which is part of the Road and Motorway Directorate of the Czech Republic.

AUGUST

> We established a cooperation with the ENET Centre, which is part of the Technical University of Ostrava, in the **Centre for Energy and Environmental Technologies** (CEET) project. The project is supported by the Technology Agency of the Czech Republic, and its aim is to find solutions for efficient transformation of alternative fuels, wastes, and by-products into recovered chemicals and useful forms of energy.

SEPTEMBER

> A two-year project to establish the **National Competence Centre in HPC** within the **EuroHPC JU** initiative launched. The aim is to share knowledge in the field of HPC across Europe and to strengthen the technological autonomy and competitiveness of the EU. In the Czech Republic, the project will establish **the National Competence Centre in HPC** and introduce support activities in this area for industry, public administration, and academia.

OCTOBER

> **The contract to build a new Euro-HPC petascale supercomputer** to be put into operation at IT4Innovations in the first half of 2021 was signed. The supplier of the supercomputer, which will serve not only the academic community but also public institutions and industrial enterprises, is Hewlett Packard Enterprise.

> The H2020 **EVEREST** project launched. The project is coordinated by IBM, consists of 10 partners, and has a duration of 36 months. The project develops a holistic approach for co-designing computation and communication in a state-of-the-art, and above all secure system for high-performance data analysis.

NOVEMBER

> Jiří Dědeček together with Edyta Tabor and Štěpán Sklenák from the J. Heyrovský Institute of Physical Chemistry of the CAS found a unique way to turn methane into methanol, for which they received the **Czech Head Invention Award**. In their research, they used IT4Innovations supercomputers, and by means of high-performance computing they predicted the results, which they eventually confirmed experimentally.

> **The 4th IT4Innovations User Conference** was held virtually with 68 participants. The conference provided information about our plans in the field of infrastructure, and new services related to our involvement in e-INFRA CZ and the LUMI consortium.

DECEMBER

> Vít Vondrák was ranked by Computerworld magazine among the **TOP personalities of 2020**. This is a mix of innovators, of start-up founders, and experienced people who have been in the IT field for a long time.

> We launched the **Visualisation and Virtual Reality Laboratory**, which will be a supporting part of the supercomputing infrastructure, and will be used to visualise 3D content using the latest technology available in large-scale 3D projection and virtual reality equipment.

IT4INNOVATIONS PROFILE

IT4Innovations National Supercomputing Center at VSB – Technical University of Ostrava is a leading research, development, and innovation centre active in the field of high-performance computing (HPC), data analysis (HPDA), artificial intelligence (AI), and their application to other scientific, industrial, and social fields, and it operates the most powerful supercomputing systems in the Czech Republic. Together with the CESNET and CERIT-SC institutions, IT4Innovations constitutes e-INFRA CZ, a strategic research infrastructure of the Czech Republic. This infrastructure is listed on the National Roadmap for Large Infrastructures for Research, Experimental Development and Innovations, prepared by the Ministry of Education, Youth and Sports of the Czech Republic.

IT4Innovations provides state-of-the--art supercomputing technologies and services to both Czech and international research teams from academia and industry. In 2020, IT4Innovations ran four supercomputers: Anselm - 94 TFlop/s, installed in the summer of 2013, Salomon - 2 PFlop/s, installed in the summer of 2015, Barbora - 849 TFlop/s, installed in the autumn of 2019, and the NVIDIA DGX-2 system specialized for artificial intelligence calculations - 130 TFlop/s and 2 PFlop/s in AI, installed in the spring of 2019. In 2020, a contract was signed for the delivery of a new petascale computing system dubbed Karolina, which will

be installed at IT4Innovations in 2021 and is built within the EuroHPC Joint Undertaking and is part of a network of eight EuroHPC supercomputers.

The key research areas of IT4Innovations include big data processing and analysis, machine learning, development of parallel scalable algorithms, solution of computationally demanding engineering problems, advanced visualization, virtual reality, modelling for nanotechnologies, and material design.

IT4Innovations research activities are executed across 5 laboratories:

> Advanced Data Analysis and Simulations Lab,
> Infrastructure Research Lab,
> Parallel Algorithms Research Lab,
> Modelling for Nanotechnologies Lab,
> Big Data Analysis Lab.

IT4Innovations also has a strong focus on cooperation with industrial enterprise, earning IT4Innovation the status of a Digital Innovation Hub registered at the European Commission level, and membership of DIHnet EU, the European network of digital innovation hubs. Digital innovation hubs are based on regional cooperation amongst multiple partners such as research organizations, industrial associations, incubators/

accelerators, and particular companies. In this context, IT4Innovations has developed a partnership with the Moravian--Silesian Innovation Centre Ostrava, and during 2020 the Digital Innovation Hub Ostrava has been established.

IT4Innovations is focused not only on providing access to state-of-the-art supercomputing systems and on activities in science, research, and innovation, but also on offering a wide range of training sessions aimed at acquiring the knowledge needed to efficiently use our supercomputing infrastructure. Furthermore, IT4Innovations is involved in educating the next generation of experts in HPC, HPDA, and AI within the Computational Sciences PhD study programme. This program is jointly guaranteed with the Faculty of Electrical Engineering and Computer Science at VSB-TUO. The centre's employees participate in ensuring education in the computationally based study programmes offered by VSB-TUO on all levels, ranging from BSc to PhD study programmes, such as computational and applied mathematics, nanotechnology, applied mechanics, and applied physics.
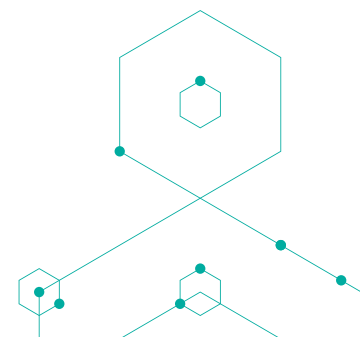
History

2011
> The foundation of IT4Innovations
> Implementation of Research Programmes
> Membership in PRACE (Partnership for Advanced Computing in Europe)

2013
> Launching of the Anselm supercomputer

2014
> Opening of the IT4Innovations building

2015
> Launching of the Salomon supercomputer
> Incorporation into the Intel® Parallel Computing Center programme

2016
> Membership in ETP4HPC (European Technology Platform for High-Performance Computing)

2018
> The Czech Republic joined the EuroHPC JU (support for building a European exascale supercomputer), in which IT4Innovations is actively involved.
> IT4Innovations became part of the H2020 POP2 Centre of Excellence and is registered by the European Commission as a DIH.

2019
> Launching of the Barbora supercomputer and the NVIDIA DGX-2 system specialized for Artificial Intelligence calculations
> Success achieved in the competition to build a EuroHPC pre-exascale supercomputing system as a member of the LUMI consortium
> Membership in BDVA (Big Data Value Association) and EUDAT CDI
> Foundation of e-INFRA CZ
> Launching of the H2020 LEXIS project, the coordinator of which is IT4Innovations
> The decision to install the Karolina petascale system in 2021 with a theoretical peak performance of 15.7 PFlop/s

2020
> Foundation of the Digital Innovation Hub Ostrava
> Signature of the contract to build the EuroHPC petascale Karolina supercomputer with a theoretical peak performance of 15.7 PFlop/s, the most powerful supercomputer in the Czech Republic
> IT4Innovations becomes the National Competence Centre in HPC

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 infra-structure in the Czech Republic, strengthening its effective use in order to increase the com-petitiveness 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.

INNOVATIVENESS

PROFESSIONALISM

IT4I Values

IT4INNOVATIONS BRAND

TEAMWORK
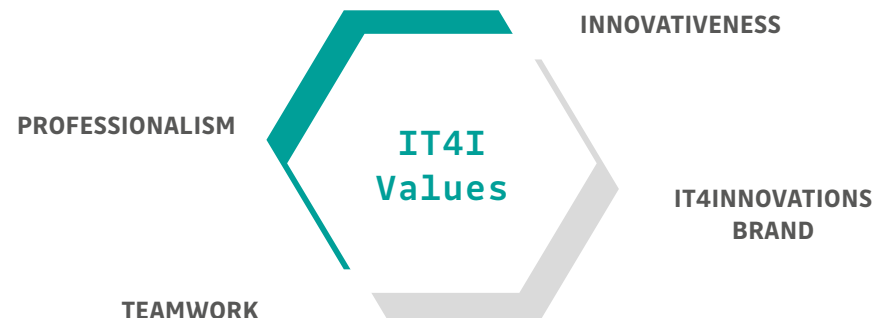
MEMBERSHIP

IT4Innovations actively participates within the EuroHPC Joint Undertaking activities, and is a member of key European infrastructures, initiatives, and associations in the field of HPC and HPDA.

PRACE
Partnership for Advanced Computing in Europe

ETP4HPC
European Technology Platform for High-Performance Computing

I4MS
ICT Innovation for Manufacturing SMEs

EUDAT
Collaborative Data Infrastructure

BDVA
Big Data Value Association

ORGANIZATIONAL STRUCTURE

IT4I Management

Vít Vondrák
Managing Director

Radim Mrázek
Administration and Finance

Branislav Jansík
Supercomputing Services

Tomáš Kozubek
Research and Development

Scientific Council	Managing Director	
Office of the Managing Director		Communication Department

ADMINISTRATION SECTION	**RESEARCH AND DEVELOPMENT**	**SUPERCOMPUTING SERVICES**
Office of the Chief Economist	Parallel Algorithms Research Lab	Division of HPC Operation and Management
Public Procurement Department	Advanced Data Analysis and Simulations Lab	Division of Hardware and Infrastructure
Administrations and Operations Department	Modelling for Nanotechnologies Lab	Department of HPC Architecture and Development
	Big Data Analysis Lab	Department of Training and Education
	Infrastructure Research Lab	

Management of IT4Innovations laboratories

Dr Jan Martinovič
Advanced Data Analysis and Simulations Lab

Dr Lubomír Říha
Infrastructure Research Lab

Dr Tomáš Karásek
Parallel Algorithms Research Lab

Prof. Jaromír Pištora
Modelling for Nanotechnologies Lab

Prof. Miroslav Vozňák
Big Data Analysis Lab

Scientific Council of IT4Innovations

CHAIRMAN

Doc. Vít Vondrák

MEMBERS

Internal

Prof. Tomáš Kozubek
Dr Branislav Jansík
Dr Jan Martinovič
Dr Lubomír Říha
Dr Tomáš Karásek
Prof. Jaromír Pištora
Prof. Miroslav Vozňák

External

Prof. Jan Holub
Faculty of Information Technology, Czech Technical University in Prague

Doc. Jiří Jaroš
Faculty of Information Technology, Brno University of Technology

Prof. Pavel Tvrdík
Faculty of Information Technology, Czech Technical University in Prague

Doc. Stanislav Hledík
Faculty of Philosophy and Science, Silesian University in Opava

Prof. Jaroslav Pokorný
Faculty of Mathematics and Physics, Charles University

Also in 2020, IT4Innovations continued its cooperation with the partners of the IT4Innovations Centre of Excellence project - the University of Ostrava, the Silesian University in Opava, Brno University of Technology, and the Institute of Geonics of the Czech Academy of Sciences. Since 2016, they have been jointly implementing the IT4Innovations Excellence in Science project, which is funded by the National Programme of Sustainability Programme II. Supervision of this project, as well as the sustainability of the IT4Innovations Centre of Excellence project is ensured by the

Supervisory Board of the IT4Innovations Centre of Excellence

CHAIRMAN

Evžen Tošenovský, Dr.h.c.

VICE CHAIRMAN

Doc. Pavel Drozd

ČLENOVÉ

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

The IT4Innovations Excellence in Science project, as well as the sustainability of the IT4Innovations Centre of Excellence project, is supervised by the Research Council of the IT4Innovations Centre of Excellence.

The Research Council of the IT4Innovations Centre of Excellence

CHAIRMAN

Doc. Vít Vondrák

MEMBERS

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The Irish Centre for High-End Computing

Prof. Petr Berka
The University of Economics in Prague

Doc. Petr Cintula
The Institute of Computer Science of the Czech Academy of Sciences

Prof. Kenneth Ruud
The Arctic University of Norway

Prof. Roman Wyrzykowski
Czestochowa University of Technology

Prof. Arndt Bode
Leibniz Supercomputing Centre of the Bavarian Academy of Sciences

Prof. Vahtang Jandieri
The University of Duisburg-Essen

Prof. Svetozar Dimitrov Margenov
The Bulgarian Academy of Sciences

Prof. Svetlana Asmuss
The University of Latvia

Employees of IT4Innovations

In 2020, the number of employees of IT4Innovations by divisions in full time equivalent (FTE) was 155.48 FTE in total, which consists of:

11%	20%	69%
Supercomputing services	Management and Administration	Research and Development

37%	Advanced Data Analysis and Simulations Lab
11%	Infrastructure Research Lab
25%	Parallel Algorithms Research Lab
19%	Modelling for Nanotechnologies Lab
8%	Big Data Analysis Lab

FINANCIAL REVIEW

## Operational and Capital Expenditures

The total expenditure of IT4Innovations amounted to CZK 227,861,000. Of this amount, non-investment (operational) expenditures and investment (capital) expenditures accounted for 91.3% and 8.7%, respectively. The largest part of the operational expenditures was made up of personnel costs, services (costs of electricity consumption, maintenance service of the operated systems and supporting infrastructure, technical and system support, etc.), overhead expenses and membership fees (to international organisations and consortia, namely PRACE, ETP4HPC, EUDAT, BDVA).

Operational expenditures structure CZK 207,943,000 in total

Investment (Capital) expenditures structure CZK 19,918,000 in total

- 37,3% Personnel costs – research labs
- 12,8% Personnel costs – management, administration
- 7,7% Personnel costs – supercomputing services
- 19,8% Services
- 17,5% Overhead costs
- 1% Fees
- 1% Small tangible fixed assets
- 0,7% International and domestic business trips (including those of invited speakers)
- 0,7% Scholarships
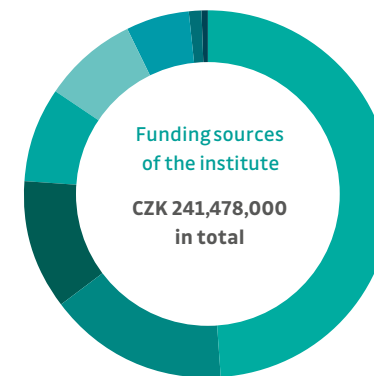- 0,6% Consumables
- 0,5% Depreciation
- 0,4% Other costs
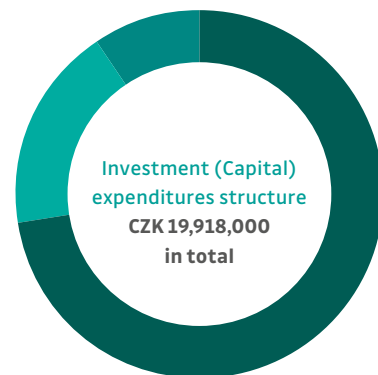
- 72,6% Tangible fixed assets – machines and equipment
- 18% Intangible fixed assets
- 9,4% Tangible fixed assets - buildings

Sources of Funding

In 2020, the overall budget of IT4Innovations was CZK 241,478,000. These resources also include unspent grant funds transferred to the earmarked fund, and profit before tax. National grants (grants from the Ministry of Education, Youth and Sports, the Technology Agency of the Czech Republic, the Grant Agency of the Czech Republic, the Ministry of Industry and Trade, and the Ministry of the Interior) accounted for the largest share of the sources of funding of operational expenditures. In addition, structural funds, international grants, the research organization development fund, internal resources, contract research and rental of computational resources, and specific research and other sources contributed to the sources of funding for operational expenditures.

Funding sources of the institute CZK 241,478,000 in total

International grants CZ 27,826,000 in total

National grants CZ 117,915,000 in total

- 49,1% National grants
- 15,7% Structural funds
- 11,5% International grants
- 8,4% Research Organization Development funds
- 8,1% Internal resources
- 5,8% Contract research and rental of computational resources
- 1,1% Specific research
- 0,3% Other
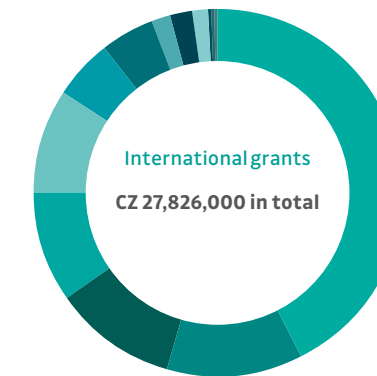
- 42,6% LEXIS
- 12% POP2
- 10,8% PRACE 6IP
- 9,7% ExaQUte
- 9,2% CloudiFacturing
- 5,3% OPENQKD
- 4,7% Expertise
- 1,8% TETRAMAX
- 1,7% EUROCC
- 1,6% PRACE 3IP
- 0,3% EVEREST
- 0,2% Superheroes4Science
- 0,1% PRACE 5IP
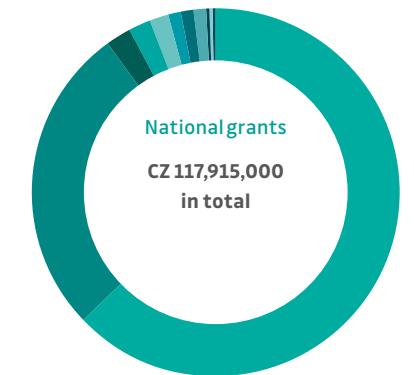
- 62,8% Large Research Infrastructures for R&D&I projects – MEYS
- 27,4% National Programme of Sustainability II – MEYS
- 2,2% Centres of Competence – TA CR
- 2% TREND – TA CR
- 1,5% Standard projects – GA CR
- 1,3% Security research of the Czech Republic – MI
- 1,1% TRIO – MIT
- 1% International grant projects evaluated on the LEAD Agency principle – GA CR
- 0,4% Support for Science and Research in the Moravian-Silesian Region – MSR
- 0,2% Individual grants – MSR
- 0,1% Researcher Mobility support within international cooperation in R&D&I – MEYS

SUMMARY OF ALL GRANTS

■ SUPERCOMPUTING SERVICES

■ RESEARCH AND DEVELOPMENT

■ EDUCATIONAL AND TRAINING ACTIVITIES

National grants

Projects supported by the Ministry of Education, Youth and Sports

Large Infrastructures Projects for Research, Experimental Development, and Innovation

- e-Infra CZ

National Programme of Sustainability II project

- IT4Innovations Excellence in Science

Grants for Specific University Research projects for 2020 – SGC

- Dynamical systems theory and its application in engineering
- Development of a Multiphysics model of an asynchronous electric motor adapted for HPC
- Experimental study and ab-initio modelling of spin lasers
- Extension of HPC Platforms for Executing Scientific Pipelines 2
- Internationalization of Doctoral Education in Molecular Physics III

- Infrastructure Research and Development of HPC Libraries and Tools II

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

- Physics of phononic interactions in solids for terahertz light generation
- Multiscale design of novel Rare Earth free permanent magnets

Projects of Operational Programme Research, Development and Education

- IT4Innovations National Supercomputing Center – Path to Exascale
- e-INFRA CZ: Modernization
- Doctoral School for Education in Mathematical Methods and Tools in HPC
- Technology for the Future 2.0

Artificial Intelligence and Reasoning

- Science without Borders 2.0

Subsidy of the Moravian-Silesian Region

- Digital Innovation Hub – Pilot Verification

Projects supported by the Grant Agency of the Czech Republic

- Space-time Boundary Element Methods for the Heat Equation
- Tailoring thermal stability of W-Cr based alloys for fusion application

Projects supported by the Technology Agency of the Czech Republic

- Personalized Medicine – Diagnostics and Therapy
- Optimization of the electrical distribution system operating parameters using artificial intelligence
- Contactless detector for partial discharges activity in medium overhead voltage powerlines
- National Centre for Energy (NCE)
- Energy system for grids
- CEET – Centre for Energy and Environmental Technologies

- Development of Expert System for Automatic Evaluation of Pathologies from Eye Images
- Research and development of a functional sample of a railway vehicle with the ability to collect data and software - a simulator with the ability to generate data for obstacle detection training in simulated conditions

Projects supported by the Ministry of Industry and Trade

- Intake and discharge objects of pump and turbine stations
- Digital twin of product within Siemens plants

Project supported by the Ministry of the Interior

- Employment of artificial intelligence into an emergency call reception

International grants

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

- PRACE-6IP – Partnership for Advanced Computing in Europe, 6th implementation phase
- LEXIS – Large-scale EXecution for Industry & Society
- EUROCC – National Competence Centres in the framework of EuroHPC
- POP2 – Performance Optimisation and Productivity 2
- CloudiFacturing – Cloudification of Production Engineering for Predictive Digital Manufacturing
- OPENQKD – Open European Quantum Key Distribution Testbed
- EXPERTISE – Experiments and High-Performance Computing

for Turbine Mechanical Integrity and Structural Dynamics in Europe

- TETRAMAX – Technology Transfer via Multinational Application Experiments
- ExaQUte – Exascale Quantifications of Uncertainties for Technology and Science Simulation
- EVEREST – dEsign enVironmEnt foR Extreme-Scale big data analytics on heterogeneous platforms

Erasmus+ projects

- SCtrain – Supercomputing knowledge partnership

International Visegrad Fund

- Superheroes4Science

SUPERCOMPUTING SERVICES

IT4Innovations is a strategic research infrastructure in the Czech Republic, and together with the CESNET and CERIT-SC institutions, it constitutes e-INFRA CZ, a strategic research infrastructure of the Czech Republic.

In 2020, IT4Innovations ran four supercomputers: Anselm (94 TFlop/s, installed in the summer of 2013), Salomon (2 PFlop/s, installed in the summer of 2015), Barbora (849 TFlop/s, installed in the autumn of 2019) and the NVIDIA DGX-2 system specialised in artificial intelligence calculations (130 TFlop/s and 2 PFlop/s in AI, installed in the spring of 2019).

In 2020, IT4Innovations continued to be actively involved in most of the activities of the EuroHPC Joint Undertaking, for which a new petascale computing system dubbed 'Karolina' will be installed in 2021 with a theoretical peak performance of approximately 15.7 PFlop/s. In particular, a contract has been signed between EuroHPC JU, Hewlett Packard Enterprise (HPE, who will supply the system), and IT4Innovations National Supercomputing Center at VSB - Technical University of Ostrava (where the new supercomputer will be located). The capabilities of Karolina will rank it amongst the most powerful supercomputers in Europe. The supercomputer is designed to comprehensively cover user requirements in solving complex scientific and industrial problems involving both classical numerical simulations and large-scale data analysis, and even the use of artificial intelligence.

IT4Innovations is also a member of the LUMI consortium (Large Unified Modern Infrastructure), bringing together Finland as the coordinator as well as Belgium, the Czech Republic, Denmark, Estonia, Iceland, the Netherlands, Norway, Poland, Sweden, and Switzerland. The aim of the consortium's cooperation is to build the EuroHPC pre-exascale LUMI supercomputing system, which will be installed in Kajaani, Finland, in the period of 2021-2022, and which will become one of the most powerful supercomputers in Europe as well as worldwide.

Technical Specifications of the Supercomputers

	Anselm	Salomon	NVIDIA DGX-2	Barbora
Put into operation	Spring 2013	Summer 2015	Spring 2019	Autumn 2019
Theoretical peak performance	94 TFlop/s	2,011 TFlop/s	130 TFlop/s 2 PFlop/s pro AI	849 TFlop/s
Operating system	RedHat Linux 64bit 6.x	CentOS 64bit 7.x	CentOS 64bit 7.x	CentOS 64bit 7.x
Compute nodes	209	1,008	1	201
CPU	2 x Intel SandyBridge, 8 cores, 2.3 / 2.4 GHz, 3,344 cores in total	2 x Intel Haswell, 12 cores, 2.5 GHz, 24,192 cores in total	2 x Intel Xeon Platinum, 24 cores, 48 cores in total	2 x Intel Cascade Lake, 18 cores, 2.6 GHz 7,235 cores in total
RAM per compute node	64 GB / 96 GB / 512 GB	128 GB / 3.25 TB (UV node)	1.5 TB DDR4, 512 GB HBM2 (16 x 32 GB)	192 GB / 6 TB fat node
GPU accelerators	23 x NVIDIA Tesla K20 (Kepler)	N/A	16 x NVIDIA Tesla V100 / 32 GB HBM2	32 x NVIDIA Tesla V100
MIC accelerators	4 x Intel Xeon Phi 5110P	864 x Intel Xeon Phi 7120P	N/A	N/A
Storage	320 TiB / home (2 GB/s), 146 TiB / scratch (6 GB/s)	500 TB / home (6 GB/s), 1,638 TB / scratch (30 GB/s)	30 TB NVMe	29 TB / home, 310 TB / scratch (28 GB/s)
Interconnection	Infiniband QDR 40 Gb/s	Infiniband FDR 56 Gb/s	8 x Infiniband or 8 x 100 GbE	Infiniband HDR 200 Gb/s

Computational Resources Allocation

The computational resources of IT4Innovations are dedicated to solving problems in research and development conducted primarily by academic and research institutions. Unused capacity can be freed up for the development of collaboration between academia and industry as well as for purely commercial use.

In 2020, IT4Innovations provided its computational resources to 184 projects within the Open Access Grant Competition and to 40 projects through the Director's Discretion scheme. A total of 267,453,643 core hours were allocated with 90% and 10% being allocated within three Open Access Grant Competitions

and through the Director's Discretion scheme, respectively. The total allocation of computational resources through the Director's Discretion scheme includes both the PRACE DECI Calls and rental in commercial sector.

Supercomputer utilisation is measured in core hours and is determined as the number of processing units (cores) used to run the simulation multiplied by the duration of the job in hours.

Open Access Grant Competitions in 2020

▢ Granted allocation

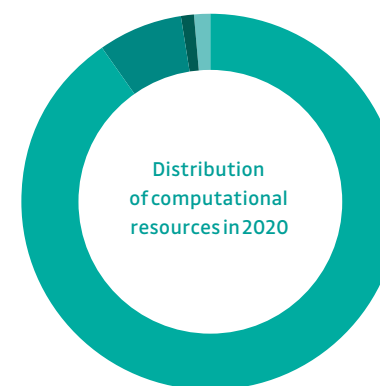◼ Difference between demand and granted allocation
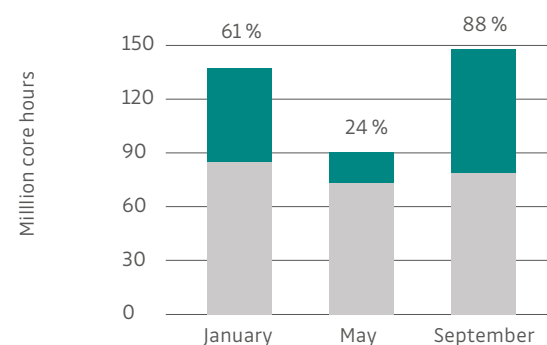
Open Access Grant Competitions

Institutions can apply for computational resources within the thrice yearly Open Access Grant Competitions. In 2020, more than 241 million core hours were allocated and distributed across 184 research projects within three Open Access Grant Competitions, enhancing Czech science.

The bulk of computational resources, i.e., 68 % and 15 %, were awarded to projects in the fields of material science and biosciences, respectively.

Given the increasing demand throughout the year 2020, the computational resources earmarked for each Open Access Grant Competition were increased from 73 up to 85 million core hours. Throughout the year, the aggregated reserved capacity was increased from 180 to 237 million core hours. In 2018 and 2019, the excess demand for core hours over the available capacity amounted to nearly 42% and 49%, respectively. In 2020, in contrast, it was 60%.

In 2020, the Allocation Committee found most of the submitted applications scientifically and technically thoroughly elaborated. However, because of insufficient capacity, the computational resources awarded to each project had to be reduced. The difference between the core hour demand and the computational resources reserved for the Open Access Grant Competitions is compensated by the reserves available through the Director's Discretion scheme as well as the IT4Innovations system administration.

Distribution of computational resources in 2020

◼ **90,4%** VGS
◼ **7,1%** PRACE DECI
◼ **1,3%** Commercial projects
◼ **1,2%** Other

Comparison of demand and granted allocation of computational resources within the Open Access Grant Competitions for 2018–2020

▢ Granted allocation

◼ Difference between demand and granted allocation
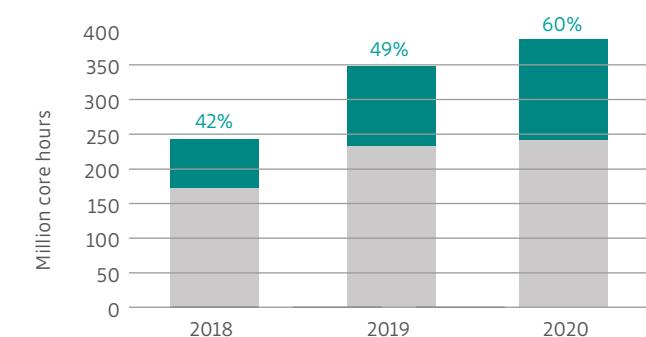
Year	Earmarked resources (corehours)	Difference between demand and earmarked computational recource	Difference between demand and granted allocation
2018	144 milionů	70%	42%
2019	180 milionů	96%	49%
2020	237 milionů	58%	60%

The Results of the Open Access Grant Competitions in 2020

Within the Open Access Grant Competitions in 2020, a total of 55 projects of applicants from VSB – Technical University of Ostrava were awarded computational resources amounting to nearly 70 million core hours. A total of 47 of these projects were led by researchers from IT4Innovations National Supercomputing Center, and the remaining projects were led by researchers from the Faculty of Ci-

vil Engineering, the Faculty of Mechanical Engineering, and the Faculty of Electrical Engineering and Computer Science.

The Czech Academy of Sciences was the second most prolific user of the IT4Innovations infrastructure. A total of 52 projects of applicants from various members of this institution were allocated more than 60 million core hours.

The projects of the Institute of Organic Chemistry and Biochemistry, the J. Heyrovsky Institute of Physical Chemistry, and the Institute of Physics received the most computational resources. CEITEC, Charles University, Brno University of Technology, the University of Ostrava, and the Czech Technical University in Prague also received allocations of at least 10 million core hours or more.
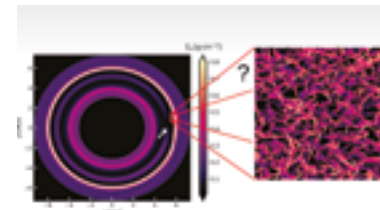
The Results of the 18th Open Access Grant Competition in Newsletter Q1/2020
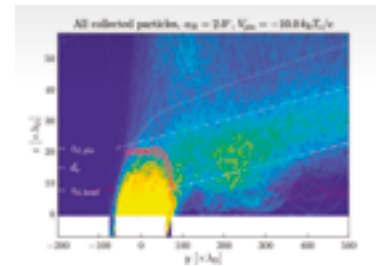
Simulation of Probe Diagnostics for COMPASS Upgrade and the project of Dr Aleš Podolník from the Institute of Plasma Physics of the Czech Academy of Sciences
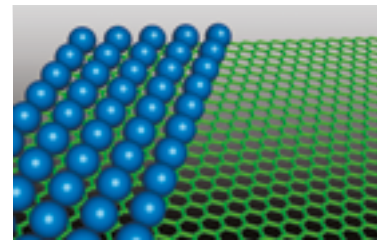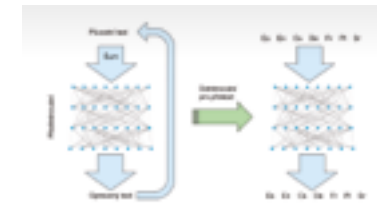
Accuracy Limits of Quantum Monte Carlo in Weak-Interaction Limit III and the project of DrMatúš Dubecký from the University of Ostrava
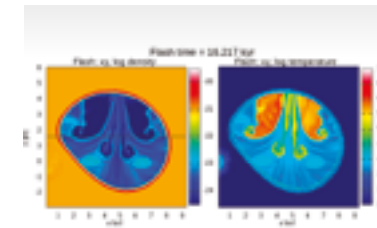
Planet Formation after Pebble Isolation and the project of Dr Ondřej Chrenko from the Astronomical Institute of Charles University

The Results of the 19th Open Access Grant Competition in Newsletter Q3/2020
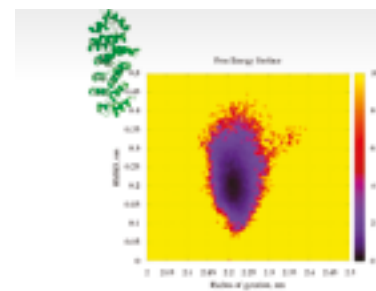
Search for New Anticancer Compounds and Investigation of their Mechanism of Action and the project of Dr Olena Mokshyna from the Institute of Molecular and Translational Medicine, Palacký University in Olomouc
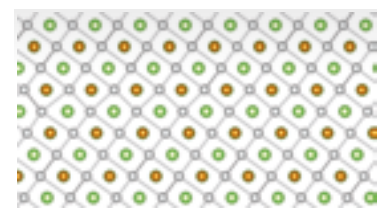
Design of a New Smart Material with Magnetic Shape Memory Effect and the project of Dr Martin Zelený from the Faculty of Mathematics and Physics, Charles University
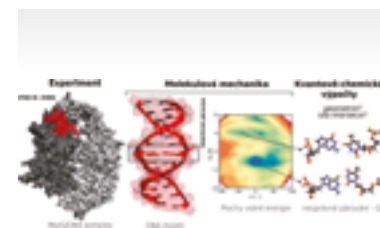
Quantum Mechanical Modelling of Mismatched DNA and the project of Dr Petr Kulhánek from CEITEC, Masaryk University
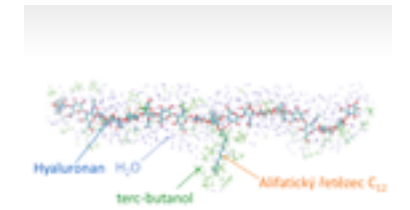
The Results of the 20th Open Access Grant Competition in Newsletter Q4/2020

Massively Multilingual and Self-supervised Neural Machine Translation for Low-Resource Languages and the project of Josef Jon from Brno University of Technology

Expansion of Supernova Driven Shells Near the Galactic Centre and the project of Dr Barnabás Barna from the Astronomical Institute of the Czech Academy of Sciences

Substituted Hyaluronan Molecules in Aqueous and Mixed Solvents and the project of Dr Marek Ingr from Tomas Bata University in Zlín

Computational resources allocated within the Open Access Grant Competitions in 2020 by institution

28,7%	VSB-TUO
24,9%	The Czech Academy of Sciences
11,8%	CEITEC
10,2%	Charles University
5,8%	Brno University of Technology
5,4%	The University of Ostrava
4,9%	CTU in Prague
2,9%	Masaryk University
2,3%	The University of Chemistry and Technology in Prague
0,6%	Tomas Bata University in Zlín
2,5%	Others

Computational resources allocated within the Open Access Grant Competitions in 2020 by scientific discipline
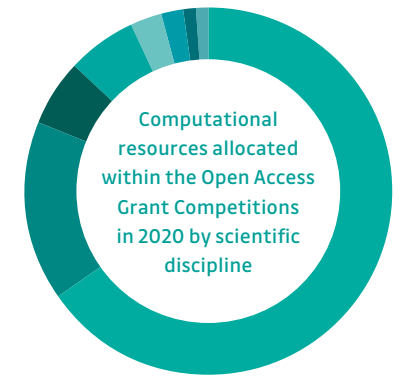
65%	Material sciences
16%	Biosciences
6%	Computer science
6%	Physics
3%	Engineering
2%	Earth sciences
1%	Astronomy
1%	Applied mathematics

Allocation of computational resources in 2018, 2019, and 2020 by scientific discipline

- Material sciences
- Biosciences
- Earth sciences
- Physics
- Engineering
- Applied mathematics
- Computational sciences
- Astrophysics
- Informatics
- Astronomy
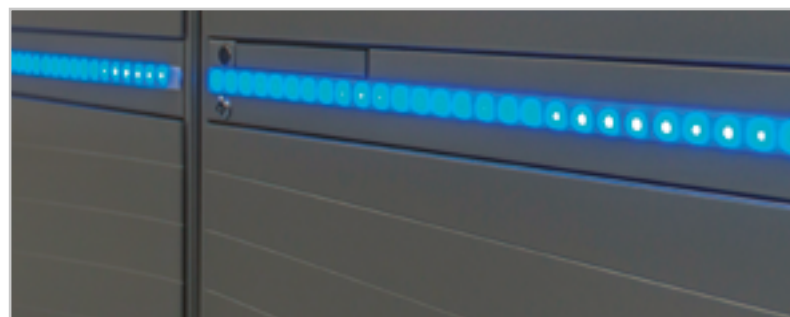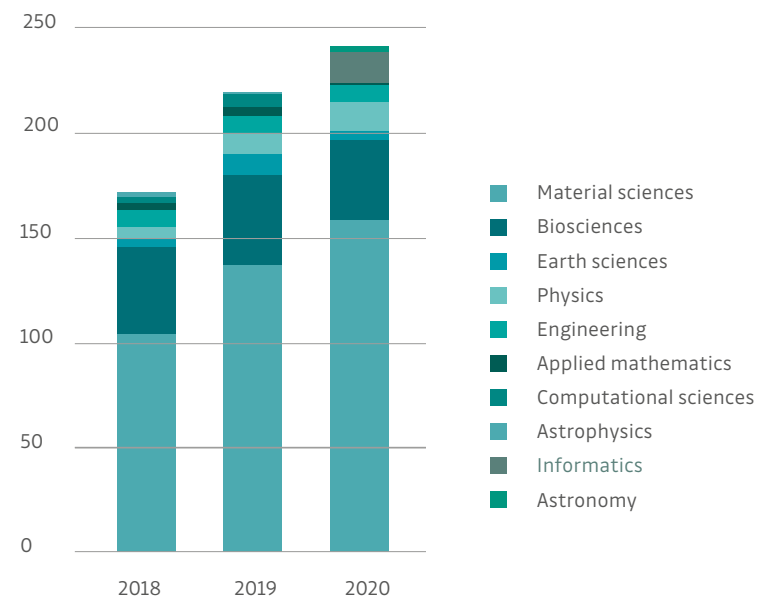
Director's Discretion

Furthermore, almost 10% of the IT4Innovations computational resources was allocated to projects within the Director's Discretion scheme. These applications can be submitted at any time. The computational resources are allocated irregularly based on evaluation by the IT4Innovations management. Any candidates can apply if Open Access Grant Competitions cannot be used. Within the Director's Discretion scheme in 2020, a total of 40 projects were allocated 26 million core hours. These projects also included those of applicants from the commercial sector, who also have the opportunity to rent the computational resources.

In 2020, the following 10 companies concluded rental agreements, amounting to approximately 3.6 million core hours:

AIRMOBIS a.s.
Bayncore Labs
Bonmedix s.r.o.
DHI a.s.
The European Space Agency
The University of Ostrava
Sotio a.s.
Ullmanna s.r.o.
The Forest Management Institute Brandýs nad Labem
Varroc Lighting systems, s.r.o.

Users of Computational Resources

In 2020, the number of active users rose to 606 in total. This is an increase of 2.5 % as compared to 2019.

In 2020, the IT4Innovations Technical Support received 1,729 queries and requests. The internal response time (24 h for the first response) was observed in 99.6 % of queries. The internal closure time, which should not be longer than 30 days, was observed in 97.57 % of queries.

Number of active users and queries and requests for technical support between 2018 and 2020

- Number of active users
- Number of queries and requests for technical support

Supercomputing Services Projects
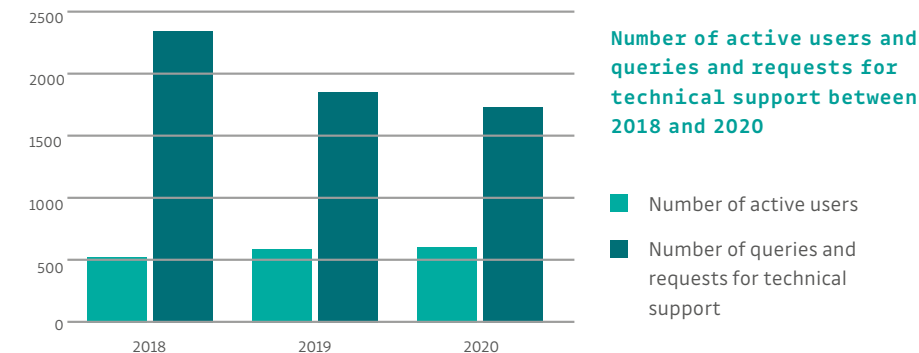
IT4Innovations is part of several national and international projects that help ensure the operation and development of supercomputing infrastructure.

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. In 2020, it was followed up by the e-Infrastructure CZ project, which brings together IT4Innovations, CESNET, and CERIT-SC. Together they form the strategic research e-infrastructure of the Czech Republic called e-INFRA CZ. This infrastructure is listed in the Roadmap of Large Research Infrastructures of the Czech Republic for Research, Experimental Development, and Innovation, which is prepared by the Ministry of Education, Youth and Sports of the Czech Republic.

The modernisation of IT4Innovations' computing capacities is funded by the Operational Programme Research, Development and Education of the MEYS, specifically from the IT4Innovations National Supercomputing Center – Path to Exascale project and the e-INFRA CZ: Modernisation project, which focuses on the modernisation and provision of necessary capacities within specific components of the e-infrastructure.

The important international projects IT4Innovations is 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 2020, already the 6th implementation phase of the project titled PRACE-6IP continues.

National Grants

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

e-Infrastructure CZ (2020–2022)

PROJECT ID LM2018140 (Large Infrastructures for Research, Experimental Development and Innovation project)

PRINCIPAL INVESTIGATOR Doc. Vít Vondrák

e-INFRA CZ is a unique e-infrastructure for research, development, and innovation in the Czech Republic, which represents a fully transparent environment providing complex capacities and resources for scientific data transfer, storage, and processing to all entities focused on research, development, and innovation across sectors. It creates a communication, information, storage, and computing platform for research, development, and innovation both at the national level of the Czech Republic and at the international level, and provides an extensive and comprehensive portfolio of ICT services, without which modern research, development and innovation could not be conducted. The main components of e-INFRA CZ include:

> high-performance national communication infrastructure;
> the national grid and cloud infrastructure;
> the most powerful and state-of-the-art supercomputing systems in the Czech Republic;
> high-capacity data storages.

Other tools and services, such as access control to ICT resources, tools to support remote collaboration, and tools to ensure secure communication and data protection, are also an essential part and an added value of this e-infrastructure, which together contribute to its efficient and diverse use.

IT4Innovations National Supercomputing Center – Path to Exascale (2017–2022)

PROJECT ID EF16_013/0001791 (Call no. 02_16_013 Research infrastructures)

PRINCIPAL INVESTIGATOR
Dr Branislav Jansík

The objective of this project is to upgrade and modernise 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. In 2018, the activities of this project were aimed at modernising the equipment and complementing the existing supercomputers with a more technologically advanced cluster similar in scope and purpose to the existing Anselm system (physically implemented in 2019 with the acquisition of the Barbora supercomputer). In 2021, 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 electro-nic structure calculations, and analysis of bioimages using HPC. In-house research is an important source of HPC expertise for IT4Innovations, which is reflected in the services the infrastructure provides to its users.

e-INFRA CZ: Modernization (2020–2022)

PROJECT ID CZ.02.1.01/0.0/0.0/18_072/0015659 (Call no. 02_18_072 Research e-infrastructures)

PRINCIPAL INVESTIGATOR
Dr Branislav Jansík

The aim of the project is to modernise and further develop the capacity of all e-infrastructure components so that the level of IT infrastructure support corresponds to the predicted requirements of the user community for the given period and at the same time to the state-of-the-art level of the field. The project focuses primarily on the complete upgrade of all layers of the common communication infrastructure and the upgrade of elements of the universal e-infrastructure capabilities for data storage and processing. An integral part of the solution will then be the optimal technological and logical interconnection of these upgraded capacities with analogous units in the European (GÉANT, EGI, EOSC, EuroHPC, ETP4HPC, EUDAT, PRACE, etc.) and global (GLIF) R&D area and, of course, with related infrastructures and entities at the national level.

International Grants

PRACE-6IP – Partnership for Advanced Computing in Europe, 6th Implementation Phase (2019–2021)

PROJECT ID 823767 (Call H2020 INFRAEDI-2018-2020)
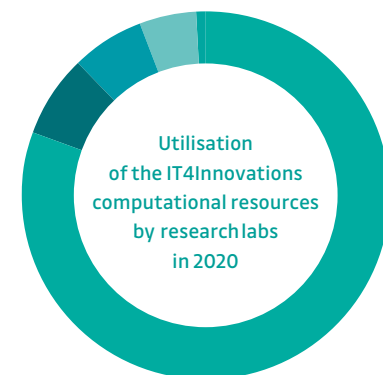
PRINCIPAL INVESTIGATOR
Doc. Vít Vondrák

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

RESEARCH AND DEVELOPMENT

IT4Innovations conducts excellent research in the field of high-performance computing, big data processing, and artificial intelligence and their application to other scientific domains and industrial practice.

The main research areas of IT4Innovations include big data processing and analysis, machine learning, development of parallel scalable algorithms, solution of computationally demanding engineering problems, advanced visualisation, virtual reality, modelling for nanotechnologies, and material design using very powerful computing and data capacities.

IT4Innovations is a research and development centre with strong international links, and as such it actively participates in all activities of the EuroHPC Joint Undertaking and in a number of prestigious international organisations (PRACE, ETP4HPC, BDVA, I4MS, HiPEAC, and EUDAT CDI). It is also involved in implementing 10 international projects funded primarily by the Horizon 2020 programme. IT4Innovations is the Coordinator of the H2020 LEXIS project as well as the National Competence Centre in HPC within the EuroCC project, and is a member of the H2020 POP2 Centre of Excellence. Moreover, IT4Innovations is involved in development of the European Space Agency (ESA) funded Urban Thematic Exploitation Platform, and has in the past participated in a number of projects supported by the FP7 and H2020 programmes such as PRACE, EXA2CT, HARPA, ExCAPE, ANTAREX, READEX, SESAME NET, and many others.

IT4Innovations research activities are executed across 5 laboratories:

ADVANCED DATA ANALYSIS
AND SIMULATIONS LAB

INFRASTRUCTURE
RESEARCH LAB

PARALLEL ALGORITHMS
RESEARCH LAB

MODELLING
FOR NANOTECHNOLOGIES LAB

BIG DATA ANALYSIS LAB

In 2020, 69 million core hours, which is 28 % of the total allocated capacity, were distributed across 55 projects of the IT4Innovations research labs. Most of the projects were submitted by the researchers from the Advanced Data Analysis and Simulations Lab, and most of the computational resources were awarded to the Modelling for Nanotechnologies Lab.

Utilisation of the IT4Innovations computational resources by research labs in 2020

■	80,8 %	NANO
■	7,1 %	ADAS
■	6,5 %	PAR
■	4,8 %	INFRA
■	0,8 %	BIG DATA

Research and Development Flagships

In 2020, IT4Innovations research and development continued to be conducted within the flagships representing IT4Innovations scientific excellence, which were selected by the Research Council of the IT4Innovations Centre of Excellence in 2018. The IT4Innovations flagships include the following three projects:

ESPRESO, Highly Parallel Finite Element Package for Engineering Simulations

PRINCIPAL INVESTIGATOR
Dr Tomáš Brzobohatý

The latest technological advances in computing have brought a significant change in the concept of new product design, production control, and autonomous systems. In the last few years, we have been witnessing a significant and considerable transition to virtual prototyping, and gradually increasing pressure to integrate large parts of the industrial sector into the fourth industrial revolution.

The main objective of the flagship is to create a robust open-source package (ESPRESO) applicable to a wide range of complex engineering simulations in areas such as mechanical engineering, civil engineering, biomechanics, and the energy industry. The open-source approach allows automatised simulation chains, based on HPC-as-a-service, such as automatised systems for shape or topological optimisation, which will be created on the top of the ESPRESO framework. In the development of new ESPRESO library components, highly scalable methods are used to take full advantage of the computational capacity of state-of-the-art supercomputers.

Material Design – Towards Reality via Exascale Computing

PRINCIPAL INVESTIGATOR
Dr Dominik Legut

As advances in HPC have been made, simulation of material behaviour has come to play a key role in our lives. This fact became even more pronounced once there was a way to perform quantum mechanical calculations to obtain the electronic structure of materials and their behaviour, and link it to many physical and chemical properties. First-principles (ab initio) calculations at present are the parameter free approach for i) verification of experiments ii) to simulate conditions or calculate material properties that are not directly accessible or measurable, and iii) to design novel materials.

Within the flagship we address fundamental and state-of-the-art topics like the design of nuclear fuel materials from radioactive compounds for generation IV nuclear reactors, ultrafast magnetisation dynamics for novel data storage, complex spintronic devices exploiting multiferroicity, and engineering applicable materials at finite temperatures and pressures, e.g., novel permanent magnets.

Advanced Data Analysis and Simulations Lab

HPC Platforms for Scientific Workflow Execution

PRINCIPAL INVESTIGATOR
Dr Jan Martinovič, Dr Stanislav Böhm and Dr Václav Svatoň

The main goal of most supercomputing centres is to lower the entry barriers to the world of HPC computing for all users from research institutes, industry, hospitals, state administration, etc. while not sacrificing execution performance. The flagship team is focused on the development of the HPC-as-a-Service concept (HaaS), which is an integral solution for HPC centres to make their HPC services available to a much broader user base. Particularly, the High-End Application Execution Platform (HEAppE Platform) is developed at IT4Innovations. This platform is not targeting one particular type of hardware for current HPC and future exascale systems, but aims to provide a solution which could be deployed to different systems and computing centres. Through this platform, all users can take advantage of the technology without an upfront investment in hardware. Simultaneously, a large portion of HPC workloads are scientific pipelines composed by domain specialists who do not have a deep knowledge of HPC technologies. Therefore, the aim is also to continue in the development of programming models capable of user-friendly workload description as well as runtime layers capable of their efficient execution in large scale distributed environments (e.g., in-house software HyperLoom), and open source the results as much as possible to increase their potential impact.

The lab specializes in advanced data analysis, research and development in the field of HPC co-design, data and cloud technologies to enhance industry and society, programing models for HPDA, Artificial Intelligence, modelling, simulation, and application of dynamical systems.

HEAD OF LAB:
Dr Jan Martinovič

NUMBER OF EMPLOYEES: 39

Significant events

> Participation in the two-year project to build **the National Competence Centre in HPC** within the EuroHPC Joint Undertaking.
> Launch of the **EVEREST** project coordinated by IBM, which aims at developing a holistic approach for co-designing computation and communication in a heterogeneous, distributed, scalable, and secure system for HPDA.
> Three EuroHPC projects with a planned launch in 2021 - **LIGATE** (LIgand Generator and portable drug discovery platform AT Exascale) coordinated by the pharmaceutical company Dompé, **ACROSS** (HPC Big Data Artificial Intelligence Cross Stack Platform Towards Exascale) coordinated by the research organisation LINKS, and **IO-SEA** (IO - Software for Exascale Architectures) coordinated by the research organisation CEA - have been successfully accepted.
> **The first version of the LEXIS** platform was developed, including the integration of pilot solutions targeting industries such as aviation, weather and climate, earthquake, and tsunami. Relevant software including distributed HPC/cloud/big-data architecture developed.
> Stanislav Böhm and Jakub Beránek presented their contribution titled "Runtime vs Scheduler: Analyzing Dask's Overheads" as part of the workshop session at the SC20 conference.
> Evaluation of the R&D output by mark 1 within the RIV 2017+ Methodology+ - Golasowski, M.; Rapant, L.; Martinovič, J.; Slaninová, K.: Autotuned Probabilistic Time Dependent Routing.

Selected publications

> Haase, Robert, Tomancak, et al.: *CLIJ – Fiji library for GPU-based image processing „CLIJ: GPU-accelerated image processing for everyone."* Nature Methods 17.1 (2020): 5–6., IF: 30.822.
> Praks, P., & Brkić, D.: *Accurate and Efficient Explicit Approximations of the Colebrook Flow Friction Equation Based on the Wright-Function: Reply to the Discussion by Majid Niazkar.* Mathematics, 2020, 8(5), 796, IF: 1.747.
> Lampart M., Zapomel J.: *Dynamics of a non-autonomous double pendulum model forced by biharmonic excitation with soft stops.* Nonlinear Dynamics 2020; 99: 1909–1921. IF: 4.867.
> Buchlovská Nagyová J., Jansík B., Lampart M.: *Detection of embedded dynamics in the Györgyi-Field model.* Scientific Reports (Nature Publisher Group) 2020; 10:21030. IF: 3.998.
> Tomcala J.: *New Fast ApEn and SampEn Entropy Algorithms Implementation and Their Application to Supercomputer Power Consumption.* Entropy, 5 Aug 2020, 22(8), 863. doi:10.3390/e22080863. IF: 2.53.

Infrastructure Research Lab

The lab specialises in acceleration of parallel applications, code analysis, performance and scalability optimisation as well as application energy-efficiency optimisation, development of services provided to infrastructure users, image processing, scientific data visualisation, and virtual reality.

HEAD OF LAB:
Dr Lubomír Říha

NUMBER OF EMPLOYEES: 12 FTE

Significant events:

> Participation in the two-year project to build **the National Competence Centre in HPC** within the EuroHPC Joint Undertaking.

> Approval of **the SCALABLE** (SCAlable LAttice Boltzmann Leaps to Exascale) and **EUPEX** projects by EuroHPC JU, which will start in 2021 or 2022.

> Developing **Rendering-as-a-Service** (RaaS) that enables users outside of High Performance Computing to use the cluster infrastructure for Blender rendering.

> The registered **MERIC** software received a high evaluation (2) in the RIV2107+ Methodology.

> Successful development of a new method for rendering large-scale scenes using multi-GPU systems such as DGX-1 and 2 and its implementation into CyclesPhi.

> Cooperation with VRgineers and CESNET leading to the development of a platform for remote interactive rendering using an HPC infrastructure for VR glasses with a resolution of up to 8k.

> Preparation of the PTC course titled Energy Efficiency in HPC and the Parallel Visualization of Scientific Data using Blender course.

> Cooperation within the international **HPC PowerStack** initiative, the objective of which is standardisation in the field of measurement, control, and optimisation of computing infrastructure energy consumption.

Selected publications:

> Wu X., Aniruddha M., Siddhartha J.; Vysocky O., Jophin J., Bartolini A., Riha L., Gerndt M., Taylor V., Bhalachandra S.: *Toward an End-to-End Auto-tuning Framework in HPC PowerStack;* Proceedings – IEEE International Conference on Cluster Computing, ICCC 2020; s.473–483.

> Kjeldsberg P.G., Schöne R., Gerndt M., Riha L., Kannan V., Diethelm K., Sawley M.-Ch., Zapletal J., Gocht A., Reissmann N., Vysocky O., Kumaraswamy M., Nagel W.: *Run-time exploitation of application dynamism for energy-efficient exascale computing;* System-Scenario-based Design Principles and Applications; Springer, s.113–126.

Parallel Algorithms Research Lab

The lab is focused on high-quality basic and applied research in the field of development of scalable algorithms and HPC libraries, numerical modelling, engineering simulations, and high-performance molecular simulations.

HEAD OF LAB:
Dr Tomáš Karásek

NUMBER OF EMPLOYEES: 26 FTE

Significant events

> Coordination and active involvement in a two-year project to build a **National Competence Centre in HPC** within the EuroHPC Joint Undertaking.

> Development of libraries for molecular simulations and their use in scientific computing: **MULTIDYN** (non-adiabatic molecular dynamics).

> Continuation of the **BESTHEA** library development within the joint Czech-Austrian project "Space-Time Boundary Element Methods for the Heat Equation" (Czech Science Foundation and the Austrian Science Fund).

> The **ESPRESO** library has been extended to include solutions to harmonic analysis problems using the FETI-H method.

> **Collaborative research** with the Siemens s.r.o. and SIGMA GROUP a.s. companies

Selected publications

> Van de Steen C., Benhenni M., Kalus R., Cosic R., Gadea F. X., Yousfi M.: *Relaxation of electronic excitations in Kr2+ ions in cold krypton plasma.* Plasma Sources Science & Technology, 2020, vol. 29, IF: 3.193.

> Lukáš D., Of G., Zapletal J., Bouchala J.: *A boundary element method for homogenization of periodic structures.* Mathematical Methods in the Applied Sciences, 2020, vol. 43, pp 1035–1052, IF: 1.626.

> Nevrly V., Dostal M., Klecka V., Bitala P., Valek V., Vasinek M., Blejchar T., Suchanek J., Zelinger Z., Wild J.: *TDLAS-based in situ diagnostics for the combustion of preheated ultra lean dimethyl ether/air mixtures.* Fuel, 2020, vol. 263, IF: 5.578.

> Liu X., Fecko P., Fohlerova Z., Karasek T., Pekarek J., Neuzil P.: *Parylene micropillars coated with thermally grown SiO2.* Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronic, 2020, vol. 38, IF: 1.511.

> Vítek A., Arismendi-Arrieta Daniel J., Sarmanova M., Kalus R., Prosmiti R.: *Finite Systems under Pressure: Assessing Volume Definition Models from Parallel-Tempering Monte Carlo Simulations.* Journal of Physical Chemistry A, 2020, vol. 124, pp 4036–4047, IF: 2.6.

> Mrovec M., Berger J.A.: *A diagonalization-free optimization algorithm for solving Kohn-Sham equations of closed-shell molecules.* Journal of Computational Chemistry, vol.42, pp 492–504, 2021, IF: 2.976.

Modelling for Nanotechnologies Lab

Big Data Analysis Lab

The laboratory focuses on optical diagnostics, material design, development of special surfaces for nano-optics, and modelling and design of nanocomposites.

HEAD OF LAB:
Prof. Jaromír Pištora
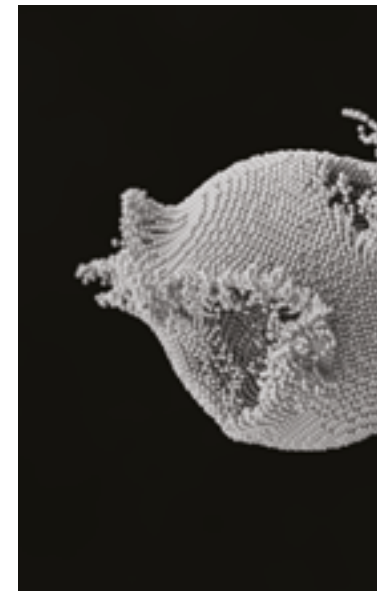
NUMBER OF EMPLOYEES: 15 FTE

Significant events

> Start of the H2020 **s-NEBULA** project, which focuses on the development of new spin-based THz building blocks for generation and detection of terahertz waves as well as advanced terahertz applications.

> Defence of Martin Mičica's dissertation at VSB-TUO and l'Université de Lille 1, France, before the joint Czech-French committee, on the dissertation topic Solid-state terahertz laser material based on molecular crystals.

> Pierre Koleják won 1st place at the 11st Czech-Slovak Student Scientific Conference in Physics (11st CSSSVR 2020) for the best diploma thesis in the Condensed Matter Physics category.

> Daniel Vala won 2nd place at the 11st Czech-Slovak Student Scientific conference in Physics (11st ČSSVR 2020) for the best diploma thesis in the Theoretical Physics category.

Selected publications

> Nieves P., Arapan S., Kadzielawa A.P., Legut D.: MAELASviewer: *An Online Tool to Visualize Magnetostriction.* Sensors 20, (2020), 6436; DOI:10.3390/s20226436, IF: 3.275.

> Arapan S., Nieves P., Herper H.C., Legut D.: *Computational screening of Fe-Ta hard magnetic phases.* Phys. Rev. B 101, 014426 (2020), DOI: 10.1103/PhysRevB.101.014426, IF: 3.575.

> Baldini E., Belvin C. A., Rodriguez-Vega M., Ozel I.O., Legut D., Kozłowski A., Oleś A. M., Parlinski K., Piekarz P., Lorenzana J., Fiete G.A., and Gedik N.: *Discovery of the soft electronic modes of the trimeron order in magnetite.* Nature Phys. 16, 541 (2020), DOI: 10.1038/s41567-020-0823-y, IF: 19.256.

> Wang T., Legut D., Fan Y., Qin J., Li X., Zhang Q.: *Building fast diffusion channel by constructing metal sulfide/metal selenide heterostructures for high-performance sodium ion batteries anode.* Nano Letters. 20, 6199-6205 (2020), DOI: 10.1021/acs.nanolett.0c02595, IF: 11.238.

> Silber R., Král D., Stejskal O., Kubota T., Ando Y., Pištora J., Veis M., Hamrle J., Kuschel T.: *Scaling of quadratic and linear magnetooptic Kerr effect spectra with L21 ordering of Co2MnSi Heusler compound.* Appl. Phys. Lett. 116, 262401 (2020); DOI: 10.1063/5.0008427, IF: 3.597.

> Drong M., Fordos T., Jaffres H.Y., Perina J., Jr., Postava K., Pistora J.,

> Drouhin H.J.: *Local and mean field approaches for modeling semiconductor spin lasers.* J. Opt. 22 (2020) 055001. DOI: 10.1088/2040-8986/ab7d8a, IF: 2.379.

> Svoboda L., Bednar J., Dvorsky R., Rybkova Z., Malachova K., Henych J., Matysek D., Nemeckova Z.: *Novel synthesis of Ag@AgCl/ZnO by different radiation sources including radioactive isotope 60 Co: Physicochemical and antimicrobial study.* Appl. Surf. Sci. 529 (2020) 147097, DOI: 10.1016/j.apsusc.2020.147098, IF: 6.182.

The lab focuses on network security, the Internet of Things, big data analytics, speech processing, and applications of artificial intelligence in complex systems.

HEAD OF LAB:
Prof. Miroslav Vozňák

NUMBER OF EMPLOYEES: 8 FTE

Significant events

> Research on robotic arm trajectory optimisation within **the Artificial Intelligence and Reasoning** project of the OP VVV Call Excellent Research Teams, together with the Czech Technical University in Prague and the University of West Bohemia in Pilsen.

> Successful completion of **the Secure IoT Gateway** project together with the CESNET association as part of the programme focused on security research for the needs of the state, funded by the Ministry of the Interior of the Czech Republic.

> As part of the **TETRAMAX** project, the creation of an IoT network in the city of Klaipeda, in which a foreign partner operates sensors for industrial applications.

> Successful completion of the Ministry of Industry and Trade project to develop a portfolio of IoT products, and registration of four prototypes: a parking sensor, a forestry sensor, a water meter, and a fire sensor.

> Within the H2020 **OpenQKD p**roject, implementation of key management in the quantum network simulator we are developing.

Selected publications

> Drungilas D., Kurmis M., Lukosius Z., Jakovlev S., Voznak M.: *An adaptive method for inspecting illumination of color intensity in transparent polyethylene terephthalate preforms (2020).* IEEE Access, 8, art. no. 9082606, pp. 83189–83198. DOI: 10.1109/ACCESS.2020.2991474, IF: 3.745.

> Mehic M., Niemiec M., Rass S., Ma J., Peev M., Aguado A., Martin V., Schauer S., Poppe A., Pacher C., Voznak M.: *Quantum Key Distribution: A Networking Perspective (2020).* ACM Computing Surveys, 53 (5), art. no. 3402192. DOI: 10.1145/3402192, IF: 7.99.

> Fazio P., Mehic M., Voznak M.: *A deep stochastical and predictive analysis of users mobility based on Auto-Regressive processes and pairing functions (2020).* Journal of Network and Computer Applications, 168, art. no. 102778. DOI: 10.1016/j.jnca.2020.102778, IF: 5.57.

> Fazio P., Tropea M., Voznak M., De Rango F.: *On packet marking and Markov modeling for IP Traceback: A deep probabilistic and stochastic analysis (2020).* Computer Networks, 182, art. no. 107464. DOI: 10.1016/j.comnet.2020.107464, IF: 3.111.

> Partila P., Tovarek J., Ilk G.H., Rozhon J., Voznak M.: *Deep Learning Serves Voice Cloning: How Vulnerable Are Automatic Speaker Verification Systems to Spoofing Trials? (2020).* IEEE Communications Magazine, 58 (2), art. no. 8999436, pp. 100 105. DOI: 10.1109/MCOM.001.1900396, IF: 11.052.

> Mehic M., Fazio P., Rass S., Maurhart O., Peev M., Poppe A., Rozhon J., Niemiec M., Voznak M.: *A Novel approach to quality-of-service provisioning in trusted relay quantum key distribution networks (2020).* IEEE/ACM Transactions on Networking, 28 (1), art. no. 8935373, pp. 168-181. DOI: 10.1109/TNET.2019.2956079, IF: 3.315.

> Krömer P., Hasal M., Nowakova J., Heckenbergerova J., Musilek P.: *Statistical and Nature-Inspired Modeling of Vehicle Flows by Using Finite Mixtures of Simple Circular Normal Distributions (2020).* IEEE Intelligent Transportation Systems Magazine, 12 (4), art. no. 9184800, pp. 182-194. DOI: 10.1109/MITS.2020.3014419, IF: 3.363.

Projects supported by the Ministry of Education, Youth and Sports

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 University of Technology, and the Institute of Geonics of the Czech Academy of Sciences. In 2020, the cooperation of these institutions continued within the National Programme of Sustainability II (IT4Innovations excellence in science) by conducting excellent research in the fields of high-performance computing, advanced data processing, artificial intelligence, and cyberphysical systems.

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

Physics of phononic interactions in solids for terahertz light generation (2019–2020)

PROJECT ID 8J19FR006

PRINCIPAL INVESTIGATOR Dr Dominik Legut

New compact solids for terahertz (THz) light generation open up new possibilities to apply terahertz radiation in wireless communication systems, security sensors and cameras, biomedicine, and spectroscopy. For subsequent application in THz frequencies ranging from 100 GHz up to 3 THz, compact high-performance coherent sources radiating under room temperature are indispensable. THz quantum cascade lasers (THz-QCL) offer a compact solution with high output performance. However, their high thermal dependence requires operation under cryogenic temperatures. On the other hand, fast development of quantum cascade lasers (QCL) in the mid-infrared spectral range allows much more efficient pumping of THz gas lasers, which is still insufficient for applications where compact THz lasers are required.

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

NEW

Multiscale design of novel Rare Earth free permanent magnets (2020–2021)

PROJECT ID: 8X20050

PRINCIPAL INVESTIGATOR Dr Dominik Legut

The proposed research is a complementary joint work of institutions: the Technical University of Ostrava (TUO), Prešov University (PU), and the Donau-University Krems (DUK). The project consists of finding novel RE-free permanent magnets by means of a detailed systematic study of Fe-Ta and Fe-Hf compounds using adaptive genetic algorithms. Best predicted structures, i.e. those exhibiting negative enthalpy (an indication of phase stability), high saturation magnetisation, and uniaxial lattice are further tested to see if they also exhibit high magnetocrystalline anisotropy, exchange integrals (J's), and temperature (Tc) of transition from magnetic to paramagnetic state. First, MAE and J's will be obtained from the quantum mechanical calculations using HPC infrastructure, followed by Tc obtained from the atomic spin dynamic calculations. The structural parameters of the most stable candidates will then be transferred to the Slovak partners to synthesise samples and to measure number of magnetic quantities like magnetisation, magnetic susceptibility etc. At the same time the Austrian

partner will perform micromagnetic simulations to determine the magnetic behaviour of given materials with respect to their texture, shape, and thickness under various thermal conditions.

Grants of MEYS for specific university research projects for 2020

Dynamical systems theory and its application in engineering

PROJECT ID SP2020/137

PRINCIPAL INVESTIGATOR Radek Halfar

The project focused on research in the field of dynamical systems and chaos theory. The emphasis was mainly on the use of these mathematical disciplines to solve current engineering problems, supporting the development of master and doctoral students in gaining experience from international events, international cooperation, and internships. Student support was provided through direct financial assistance in the form of scholarships. Further support was provided through funding for trips to international institutes and international conferences for the professional development of students and for the presentation of results achieved in the research project.

Development of a Multiphysics model of an asynchronous electric motor adapted for HPC

PROJECT ID SP2020/139

PRINCIPAL INVESTIGATOR Marek Konečný

In the project, a complex model of an asynchronous electric motor was created, which included physical phenomena such as electromagnetism, thermomechanics, fluid flow, structural mechanics, and acoustics. The computational model was created simultaneously in commercial programs and partly in the ESPRESO numerical library. Simulations were performed for individual physical models as well as a multiphysical analysis performed by means of HPC. In order to extend the ESPRESO numerical library, optimisation of FETI methods for wave propagation and harmonic analysis were developed. The project included the study and implementation of the spatiotemporal boundary element method for the heat equation and its acceleration on GPUs.

Experimental study and ab-initio modelling of spin lasers

PROJECT ID SP2020/150

PRINCIPAL INVESTIGATOR Mariusz Drong

Vertical-cavity surface-emitting lasers (spin-VCSELs) are multilayer semiconductor structures with a spin-polarised active medium consisting of quantum wells (QW) and dots (QD). In the near future, they will find applications in spintronics as spin amplifiers or, for example, in optical communication systems as ultrafast optoelectronic modulators for ultrafast data transmission.

Extension of HPC Platforms for Executing Scientific Pipelines 2

PROJECT ID SP2020/167

PRINCIPAL INVESTIGATOR Jan Křenek

This project is a follow-up to SGS's 2019 project entitled Extension of HPC platforms for executing scientific pipelines, one of the main milestones of which was the integration of HPC-as-a-Service with a workflow manager. The follow-up focused on documenting and publishing the developed solutions and extending them with new workflows. Within this project we also focused on monitoring

services and runtime workflows, application security, and the use of compression algorithms to make data transfer more efficient. The application domains were mainly in the area of traffic modelling and machine learning applications. Another objective of the project was to foster collaboration with leading research institutes and to train students at major international schools and workshops.

Internationalization of Doctoral Education in Molecular Physics III

PROJECT ID SP2020/168

PRINCIPAL INVESTIGATOR Martin Mrovec

The project built on the previous projects implemented in past years when international cooperation was established with institutions like l'Université de Toulouse III Paul Sabatier, Toulouse, France (molecular simulations, electronic structure calculations), l'Université de Paris- Est Marne-la-Vallée, Paris, France (PIMC simulations), and Instituto di Física Fundamental, Madrid, Spain (Monte Carlo simulations). The main objective of the project was to continue pursuing this cooperation as well as to extend it with new institutions, namely the HLRS High-Performance Computing Center, Stuttgart, Germany and Institut Ruđer Bošković, Zagreb, Croatia. The results achieved through the international cooperation were presented, among others, at international conferences.

Infrastructure Research and Development of HPC Libraries and Tools II

PROJECT ID SP2020/21

PRINCIPAL INVESTIGATOR Ondřej Vysocký

The project focused on the development of existing tools developed at IT4Innovations Infrastructure Research Lab, building on the previous SGS 2019/59 project. As graphics cards have become an increasingly common source of power for the world's largest supercomputers, the common theme of the project was to support the use of GPUs in the ESPRESO, Blender, and MERIC tools. Specifically, this involved implementation of the Schur complement construction on the GPU within ESPRESO, interactive rendering distributed across a set of graphic cards using a modified version of the Cycles renderer, and measuring power consumption and tuning available Nvidia GPU parameters with the MERIC library.

Projects supported by the Grant Agency of the Czech Republic

Space-time Boundary Element Methods for the Heat Equation (2019–2020)

PROJECT ID 19-29698L

PRINCIPAL INVESTIGATOR Dr Michal Merta

The project brings together experts in two related fields, numerical analysis and high-performance computing, to jointly develop fast and massively parallel methods for general discretisation of space-time boundary integral equations for the heat equation to enable adaptive mesh refinement in space and time. The developed methods will be based on clustering, which is used for discretisation with a constant time step and a fixed space mesh. To generate adaptive meshes, classical a posteriori estimate methods will be applied. Being memory-intensive, solution of global space-time problems requires the use of computing clusters. However, it also permits space-time parallelisation. An optimised and parallelised code will thus enable full performance utilisation of the existing as well as future supercomputers.

NEW
Tailoring thermal stability of W-Cr based alloys for fusion application (2020–2022)

PROJECT ID 20-18392S

PRINCIPAL INVESTIGATOR Dr Andrzej Kądzielawa

The project deals with the physical principles that will lead to an increase in the phase stability between the immiscibility and melting temperatures by means of an example of desired alloys with a self-passivation role for fusion reactor

vessels. To this end, a phase diagram of the W-Cr system will be constructed using first-principles methods and the physical properties (speed of sound, melting temperature, region of immiscibility) therefrom. Both the phase diagram and these quantities will be verified experimentally. By enriching the alloy with transition metals from the sixth period, changes in both melting and the miscibility of the phases will be achieved. The main idea of the project is to determine the change in these temperatures based on the change in the acoustic branches of the phonon spectrum (elasticity) of the added element. Using XRD analysis and RUS measurements of experimental samples, we will obtain data to provide feedback for theoretical modelling in order to develop an alloy able to withstand a "Loss of Coolant Accident". We further derive a physical model based on the Hubbard Hamiltonian to determine the effect of quantities such as entropy on the behaviour of the immiscibility region.

Projects supported by the Technology Agency of the Czech Republic

Personalized Medicine – Diagnostics and Therapy (2019–2020)

PROJECT ID TN01000013

PRINCIPAL INVESTIGATOR Dr Jan Martinovič

The PerMed Center is focused on applied research in diagnostics and therapy of rare and genetically determined diseases. The aim is to develop both personalised diagnostic methods as well as drugs which would help specific groups of patients. The approach is highly interdisciplinary, combining medicine, chemistry, biology, genetics, and bioinformatics. All research activities include molecular target validation, medicinal chemistry, biological chemistry and preclinical development, biomarkers, and DNA analyses. Results of the PerMed Center are commercialised both by licensing as well as establishment of spin-offs.

NEW
Development of Expert System for Automatic Evaluation of Pathologies from Eye Images (2020–2022)

PROJECT ID FW2020151

PRINCIPAL INVESTIGATOR Dr Kateřina Slaninová

In compliance with the TREND programme, the main objective of the project is to increase the international competitiveness of the applicant Bonmedix Holding a.s, especially by penetrating markets in the EU and USA with a newly developed service that will subsequently be certified as a medical device. The main objective will be achieved through the development and subsequent clinical

testing of the software prototype of an expert system for the automatic evaluation of pathologies from eye images in diagnosis of diabetic retinopathy. The expert system will use a computer neural network and mathematical and statistical methods to demonstrate its ability to automatically evaluate pathologies on eye images at a similar quality to fully qualified medical staff, and this ability will then be clinically validated on real data.

NEW
Research and development of a functional sample of a railway vehicle with the ability to collect data and software - a simulator with the ability to generate data for obstacle detection training in simulated conditions (2020–2022)

PROJECT ID FW01010274

PRINCIPAL INVESTIGATOR Dr Petr Strakoš

The main objective of the project is to develop a functional sample of a railway vehicle detecting obstacles in the driving profile using a set of HW sensors, a sophisticated architecture for data processing, and artificial intelligence tools for final identification of obstacles and their interpretation to the locomotive driver. As a key support for development and optimisation of the detection system, the project includes development of a software simulator for virtualisation of

railway conditions as well as implementation of test rides in a laboratory environment.

Projects supported by the Ministry of Industry and Trade

Intake and discharge objects of pump and turbine stations (2018–2021)

PROJECT ID FV30104

PRINCIPAL INVESTIGATOR Dr Tomáš Brzobohatý

The project objectives are as follows: 1. Development and verification of a multiphase numerical computational model utilising cavitation and free surface. 2. Experimental research of flow in the model intake and discharge objects, and the creation of an experimental results database for verification of numerical computational models. 3. Utilisation of shape optimisation for the design of new pump and turbine stations, including intake and discharge objects.

Digital twin of product within Siemens plants (2019–2022)

PROJECT ID CZ.01.1.02/0.0/0.0/17_176/0 015651

PRINCIPAL INVESTIGATOR Dr Tomáš Brzobohatý

The aim of the project is the research and development of the digital twin product at Siemens, s.r.o. The project will be divided into two parts with the first part, the research and development of the digital twin product and an asynchronous electric motor, being conducted at the Siemens branch s.r.o. Elektromotory Frenštát.

Subsidy of the Moravian--Silesian Region

NEW
Digital Innovation Hub – Pilot Verification (2020–2021)

PROJECT ID 08183 2019 RRC (S516/20-96100-01RN)

PRINCIPAL INVESTIGATOR Martin Duda

Financial support from the Moravian--Silesian Region for the provision of discounted services related to the use of the computing capacity of the IT4Innovations National Supercomputing Center. This support is intended for small and medium-sized enterprises with a registered office or branch in the Moravian-Silesian Region and is provided under a de minimis regime for the period 2020-2021. The aim of this support is to enable progressive small and medium-sized enterprises, including start-ups, to use supercomputing (HPC) technologies and

expertise for the development of their business.

Projects of Operational Programme Research, Development and Education

IT4Innovations National Supercomputing Center – Path to Exascale (2017–2022)

PROJECT ID EF16_013/0001791

PRINCIPAL INVESTIGATOR Dr Branislav Jansík

The objective of the project is, among others, to extend IT4Innovations in--house research in the three following fields: 1) Modelling of photonic and spin-photonic structures, design of progressive materials based on electronic structure calculations, and bioimage analysis using HPC. 2) Use of approximations involving many-body effects (MB) in electrons, the inclusion of temperature effects in computational methods, in particular anharmonic lattice vibration effects, and thus the possibility to study materials in near-realistic conditions, and phenomena at the mesoscale level (i.e. those including tens of thousands to millions of atoms, such as the effect of interfaces, dislocations, and other defects on material properties, as these exist in real materials and often limit their use).

3) Creation of a globally unique platform for the analysis of biological and bio-medical image data using high-performance computing (HPC) infrastructure based on the open-source Fiji platform. 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 Artificial Intelligence 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 stems from 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.

Projects with IT4Innovations participation

Optimization of the electrical distribution system operating parameters using artificial intelligence (2019–2021)

PROJECT ID TJ02000157

PRINCIPAL INVESTIGATOR Jan Vysocký (ENET, VSB-TUO)

The objective of the project is to create an optimisation system and a strategy for optimising the operation of the electrical distribution system (DS). The control optimisation system will consist of a program and an interface. The program will set various DS elements to optimise the DS operation in multiple ways (i.e., operation with minimal cost, with maximum reliability, etc.). Optimal DS configuration will be achieved, for example, by changing network topology or controlling local active and reactive power sources. The interface will allow the proposed program to be included in the existing dispatching control structures of the DS. The optimisation strategy will describe all the hardware and software innovations that need to be performed

to maximise the DS management capabilities.

Contactless detector for partial discharges activity in medium overhead voltage powerlines (2019–2021)

PROJECT ID TJ02000031

PRINCIPAL INVESTIGATOR Dr Jan Fulneček (ENET, VSB-TUO)

The aim of this project is the development of an on-line insulation diagnostics tool for high-voltage overhead powerlines with covered conductors. A contactless sensor will be designed and constructed for test operation. This sensor will be used to record partial discharge patterns inside and on the surface of a covered conductor. An algorithm for automatic detection of partial discharge patterns in acquired signals will be created. Based on the presence of the partial discharge pattern in the acquired signal, the algorithm automatically evaluates the insulation state of the covered conductor. This goal will be met by the end of the project duration.

National Centre for Energy (NCE) (2019–2020)

PROJECT ID TN01000007

PRINCIPAL INVESTIGATOR Prof. Stanislav Mišák (ENET, VSB-TUO)

The objective of the National Centre for Energy (NCE) is to stimulate long-term cooperation among the leading research organisations and major application entities in the power industry. Consequently, unique infrastructures and the know-how of expert teams of the existing research centres will be shared through the implementation of joint applied research projects. The research agenda of the NCE is in line with the National RIS3 Strategy and focuses on new technologies leading to increasing efficiency, safety, and reliability of existing energy units, efficient deployment and operation of decentralised sources of energy, use of alternative fuels to secure mineral resources independence and the energy self-sufficiency of the Czech Republic, and power grids safety and security.

Energy system for grids (2019–2023)

PROJECT ID TK02030039

PRINCIPAL INVESTIGATOR Prof. Stanislav Mišák (ENET, VSB-TUO)

The aim of the project is the development of a new system solution for energy flow control in the energy platform of a Sophisticated Energy System (SEN) on the level of distribution networks to supply energy platforms of municipalities, towns, and microregions. The SEN will be supported by sophisticated control methods and

prospective technologies to increase its security, reliability, raw material self-reliance, and energy self-sufficiency, while maximising the exploitation of decentralised, particularly renewable sources of energy. The objective is to ensure the readiness for a change in the energy system control concept after implementing the EU Winter Package, in compliance with the National Action Plan for Smart Grids and the updated State Energy Conception within the 5-year implementation of the project.

Employment of artificial intelligence into an emergency call reception (2019–2022)

PROJECT ID VI20192022169

PRINCIPAL INVESTIGATOR Petr Berglowiec

This project focuses on the deployment of artificial intelligence technologies for automated reception and processing of emergency calls by means of a voice chat-bot. Advances in speech analytics, semantic analysis, dialogue management, and voice synthesis are expected, including integration of geographical data. The output is a functional demonstrator working with real telephone calls under the condition of close deployment in an Integrated Rescue System (IRS), and recommendations for the system integration and its further development towards IRS automation.

International Grants

EXPERTISE – Models, Experiments and High-Performance Computing for Turbine Mechanical Integrity and Structural Dynamics in Europe (2017–2021)

PROJECT ID 721865 (Call no. H2020-MSCA-ITN-2016)

PRINCIPAL INVESTIGATOR Prof. Tomáš Kozubek

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

TETRAMAX – Technology Transfer via Multinational Application Experiments (2017–2021)

PROJECT ID 761349 (Call no. H2020-ICT-2016-2)

PRINCIPAL INVESTIGATOR Prof. Miroslav Vozňák

Within this project, the "Smart Anything Everywhere" initiative will be implemented in the field of Customized Low

Energy Computing for cyber physical 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 (Call no. H2020-FOF-2017)

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 manufacturing companies and thus increase their competitiveness. This project aims at optimisation of production processes and productivity of companies using HPC-based modelling and simulation as cloud services.
www.cloudifacturing.eu

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

PROJECT ID 800898 (H2020-FETHPC-2016-2017)

PRINCIPAL INVESTIGATORS: Dr Tomáš Karásek and Dr Jan Martinovič

The objective of ExaQUte, a three-year project, is to develop new methods that allow the solution of complex engineering 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 optimising geometrically complex civil engineering structures. IT4Innovations will participate in deploying the Hyperloom and COMPSs tools using high-performance computing systems, their configuration, and optimisation. Our participation also includes testing of robust algorithms for shape optimisation of wind-loaded structures.
www.exaqute.eu

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

PROJECT ID 824080 (H2020-INFRA-EDI-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, identify erroneous parts of codes, and make recommendations of optimisation methods resulting in increased performance and better scalability of a given application.
www.pop-coe.eu

LEXIS – Large-scale EXecution for Industry & Society (2019–2021)

PROJECT ID 825532 (H2020-ICT-2018-2020)

PRINCIPAL INVESTIGATOR Dr Jan Martinovič

The objective of this project, for which IT4Innovations is the coordinator, is to develop an engineering platform using state-of-the-art technologies such as high-performance computing, big data, and cloud services. The benefits coming out of the LEXIS projects will be demonstrated via three pilot tests suitable for industrial fields such as aerospace, weather and climate, and earthquakes and tsunami.
www.lexis-project.eu

OPENQKD – Open European Quantum Key Distribution Testbed (2019–2022)

PROJECT ID 857156 (H2020-SU-ICT-2018-2020)

PRINCIPAL INVESTIGATOR Prof. Miroslav Vozňák

The project aims at establishing a testbed for a highly secure network using the principles of quantum mechanics for key distribution. It has been the largest implementation of QKD (Quantum Key Distribution) in Europe so far. The role of IT4Innovations lies primarily in three areas. The first is a real use case of HPC via QKD between IT4Innovations and Poznan Supercomputing and Networking Center (PSNC). The second is participation in the development and implementation of key management. The third is a simulation of QKD use cases of all partners in the project as well as the improvement of an open-source QKD simulator, which is being developed open source in Ostrava. For the simulations, the computational resources of the IT4Innovations National Supercomputing Center are used.
www.openqkd.eu

NEW
EUROCC – National Competence Centres in the framework of EuroHPC (2020–2022)

PROJECT ID 951732 (H2020-JTI-Euro-HPC-2019-2)

PRINCIPAL INVESTIGATOR Dr Tomáš Karásek

The EuroCC project will bring together expertise to create a European network of National Competence Centres in HPC in 31 European countries to provide a portfolio of services for the needs of industry, academia, and public administration. Its aim is to strengthen expertise and skills in high-performance computing, data analytics, and artificial intelligence, and to bridge the existing national gaps in the use of these technologies.
www.eurocc-project.eu

NEW
EVEREST – dEsign enVironmEnt foR Extreme-Scale big data analytics on heterogeneous platforms (2020–2023)

PROJECT ID 957269 (H2020-ICT-2018-20 / H2020-ICT-2020-1)

PRINCIPAL INVESTIGATOR Dr Kateřina Slaninová

The project aims at developing a holistic approach for co-designing computation and communication in a state-of-the-art

and, primarily, secure system for HPDA. This is achieved by simplifying the programmability of heterogeneous and distributed architectures through a "data-driven" design approach, the use of hardware-accelerated AI, and through efficient monitoring of the execution with a unified hardware-software paradigm. The project will validate its approach through three case studies, a weather-based prediction model, an air quality monitoring application, and a traffic modelling framework for smart cities.
www.everest-h2020.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 2020 included collaboration with these companies:

Bayncore Labs Limited:
2 cooperation projects

National Cyber and Information Security Agency

Josef Dušek

EDUCATIONAL AND TRAINING ACTIVITIES

Study Programmes

IT4Innovations together with the Faculty of Electrical Engineering and Computer Science of VSB-TUO run the Computational Sciences PhD study programme. Unique within the Czech Republic, this programme is focused on the use of HPC, HPDA, and AI in science and industry. At the end of the year 2020, there were 25 students studying within this as well as the eponymous all-university programme. The Computational Sciences PhD study programme is part of the MathInHPC Doctoral School, bringing together leading Czech workplaces focused on research in the field of HPC methods and their applications. Its students thus have an opportunity to get in touch with prominent experts from the Doctoral School partner institutions such as the Faculty of Mathematics and Physics of Charles University in Prague and the Institute of Mathematics of the CAS.

IT4Innovations is also strongly engaged in teaching within the Computational and Applied Mathematics MSc study programme, which is guaranteed by the Department of Applied Mathematics at the Faculty of Electrical Engineering and Computer Science of VSB-TUO, in particular within the Computational Methods and HPC specialisation. Furthermore, IT4Innovations is also significantly involved in teaching at all levels of the Nanotechnology study programme guaranteed by the Faculty of Materials Science and Technology.

Educational Activities

IT4Innovations supports the scientific community as well as its users by organising 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 the fields of HPC, HPDA, and AI.

In 2020, IT4Innovations organised 8 educational events attended by 249 participants.

Having been awarded **PRACE TRAINING CENTER** (PTC) status in 2017, IT4Innovations organised six courses under the auspices of PRACE in 2020. Among others, these courses included:
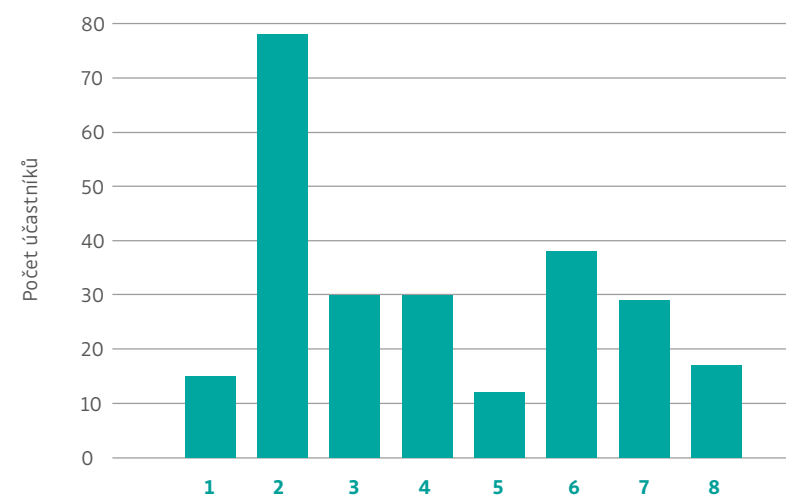
> **ENERGY EFFICIENCY IN HPC** (Lubomír Říha, Ondřej Vysocký, Andrea Bartolini, Daniele Cesarini, Robert Schönke), which focused on energy consumption and energy efficiency of HPC systems.

> **PARALLEL VISUALIZATION OF SCIENTIFIC DATA USING BLENDER** (Petr Strakoš, Milan Jaroš, Alena Ješko), which focused on visualisation of simulated data using the modelling Blender tool.

Having the status of **NVIDIA DEEP LEARNING INSTITUTE Ambassador**, in 2020 IT4Innovations also offered the following practical courses for developers and researchers wishing to solve complex problems using deep learning:

> **NVIDIA AI & HPC ACADEMY** a three full-day NVIDIA Deep Learning Institute-certified training session, during which attendees had the opportunity to learn more about artificial intelligence (AI) development and high-performance computing (HPC) for NVIDIA GPUs. The following courses were also included: FUNDAMENTALS OF DEEP LEARNING FOR COMPUTER VISION, FUNDAMENTALS OF ACCELERATED COMPUTING WITH CUDA C/C++, and FUNDAMENTALS OF ACCELERATED COMPUTING WITH OPEN ACC (Georg Zitzlsberger).

> **FUNDAMENTALS OF DEEP LEARNING FOR MULTIPLE DATA TYPES** (Georg Zitzlsberger) about a combination of convolutional and recurrent neural networks, enabling the generation of effective descriptions of content in images and video clips using the TensorFlow dataset and Microsoft Common Objects in Context (COCO).

> **FUNDAMENTALS OF DEEP LEARNING FOR MULTI-GPUS** (Georg Zitzlsberger) about the possibility of using multiple GPUs for deep learning, which can significantly reduce time, thus allowing complex problems to be solved.

Educational activities in 2020

Počet účastníků (y-axis: 0, 10, 20, 30, 40, 50, 60, 70, 80)
Categories: 1, 2, 3, 4, 5, 6, 7, 8

1. Energy Efficiency in HPC (PTC)
2. Fundamentals of Deep Learning for Computer Vision
3. Fundamentals of Accelerated Computing with CUDA C/C++ (PTC)
4. Fundamentals of Accelerated Computing with Open ACC (PTC)
5. Parallel Visualization of Scientific Data using Blender (PTC)
6. Fundamentals of Deep Learning for Multiple Data Types (PTC)
7. Fundamentals of Deep Learning for Multi-GPUs (PTC)
8. Introduction to High Performance Computing

PRACE Summer of HPC

Already for the 8th time, the Partnership for Advanced Computing in Europe (PRACE) allowed students to participate in a summer internship in European supercomputing centres, this time virtually. This opportunity was exploited by 50 students who were involved, together with their mentors, in 24 projects. IT4Innovations hosted two of them.

Denizhan Tutar, a PhD student of Computational Science and Engineering at Istanbul Technical University, was involved in the project entitled Development of a Visualization Tool for Data from Molecular Simulations under the supervision of Martin Beseda and Rajko Cosic.

Andres Vicente Arevalo, an astrophysics student at Universidad de La Laguna on Tenerife, worked on the project entitled Object Detection Using Deep Neural Networks – AI from HPC to the Edge under the supervision of Georg Zitzlsberger and Martin Golasowski.

Educational Projects

Projects of the 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_018/00 02713 (Call no. 02_16_018)

PRINCIPAL INVESTIGATOR Prof. 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 modernise and internationalise one of the doctoral programmes 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 de Toulouse III Paul Sabatier, France).

Technology for the Future 2.0 (2019–2022)

PROJECT ID CZ.02.2.69/0.0/0.0/18_058/0 010212 (Call no. 02_18_058)

PRINCIPAL INVESTIGATOR FOR IT4INNOVATIONS Prof. René Kalus

The project aims at enhancing the quality and profile of educational activities and increasing their relevance for the labour market. It implements new forms of educational methods, establishes new study programmes, and boosts the internationalisation of the university and ties between the university and its graduates. It implements methods for increasing participation of students with special needs, as well as improving the strategy for motivating secondary school students to enrol for tertiary education studies. It enhances not only the capacities of the management personnel of higher education institutions (HEI), but also the quality of the HEI strategy management. The main objective of the project is to increase the relevance of VSB-TUO educational activities to the needs of the labour market. In practical terms this means reaching a state where the university educational activities reflect the needs and unique features of the labour market in the Moravian-Silesian Region and of all target groups.

NEW
Science without Borders 2.0 (2020–2022)

PROJECT ID CZ.02.2.69/0.0/0.0/18_053/0 016985 (Call no. 02_18_053)

PRINCIPAL INVESTIGATOR FOR IT4INNOVATIONS Prof. Tomáš Kozubek

The Science without Borders 2.0 project will facilitate the mobility of 26 researchers of diverse nationalities to and from the Czech Republic. It will thus address the insufficient level of international cooperation in research and the professional growth of human resources in research. Researchers will develop in their fields of research, transferring their knowledge to workplaces and research teams of VSB-TUO. The support is primarily directed at junior researchers with the potential to accelerate their research work.

Projects of the International Visegrad Fund

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

ERASMUS+ Projects

NEW
SCtrain – Supercomputing knowledge partnership (2020–2023)

PROJECT ID 20-203-075975 (KA203-6E6A1FFC)

PRINCIPAL INVESTIGATOR Prof. Tomáš Kozubek

The mission of this project is a methodical approach to fill gaps in current university courses and increase awareness of HPC for future professionals in science, technology, engineering, and mathematics. www.sctrain.eu

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