



# Review 2022

Our supercomputers  
support science,  
industry, and society.

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# Managing Director's Introduction

The year 2022 is over, and thus this is an excellent opportunity to look back at what the year was like. In short, it was another year lined with more achievements, big and small, which I would like to share with you in the following lines.

The cornerstone of our centre is the operation of supercomputers and the provision of computational resources not only to the scientific but also to the industrial community. The most recent additions to our data room are complementary systems consisting of multiple hardware platforms that provide access to emerging, non-traditional, and highly-specialised hardware architectures not yet common in supercomputing centres. While we are waiting for a new supercomputer, we have been providing the Czech scientific community with access to LUMI, Europe's most powerful supercomputer, since last year, thanks to our membership in the eponymous consortium. Being part of its management structure, we provide expert support to users and develop software tools such as HyperQueue, allowing users to efficiently use the available computational resources of this third most powerful supercomputer in the world. We followed up our collaboration within the LUMI consortium by submitting the LUMI-Q project to the EuroHPC JU competition for the placement and operation of a quantum computer, in which we were successful, and we hope to see this unique technology in our centre in 2024. This quantum computer will become the first-ever quantum computer in the Czech Republic.

We were also successful in the area of research projects - international projects such as EUPEX, OpenWebSearch, and BioDT were newly launched, and in 2022 we were

thus involved in a total of 15 international projects funded by Horizon 2020 and Horizon Europe programmes, including the POP2 Centre of Excellence. The National Competence Centre in HPC, whose activities in the Czech Republic are covered by our supercomputing centre, has entered its third year of operation. Among the research of our colleagues, I would like to highlight the award for the best scientific poster at SC23, the world's largest conference for HPC. Moreover, our colleagues published their discovery in biodiesel waste utilisation into a functional product, increasing the efficiency of existing biofuels in the journal Nature Communications. Last, I would like to congratulate Professor Pavel Hobza for winning the Neuron Prize in Chemistry.

Our centre does not only cooperate with academia, but also focuses part of its activities on cooperation with industry. Last year, the activities of IT4Innovations, the Faculty of Electrical Engineering and Computer Science, which are both part of VSB - Technical University of Ostrava, and the Moravian-Silesian Innovation Centre Ostrava were brought together to form the European Digital Innovation Hub Ostrava. Starting this year, it supports introducing and deploying digital technologies primarily in small and medium-sized enterprises to promote their competitiveness.

Education is also an integral part of our activities offered to our users and the wider professional public. Last year, we organised an incredible 17 courses and workshops, attracting almost 600 people. At the same time, we launched EUMaster4HPC, a unique pan-European MSc study programme for education in high-performance computing. I am delighted that we have been part of it since the beginning and can also offer this study programme to students from the Czech Republic.

However, last year was about more than just positive events. For the first time in the history of our centre, we were forced to shut down all systems for several weeks due to the collapse of our electricity supplier and the subsequent enormous price of electricity. Fortunately, we managed to resolve this crisis thanks to an extraordinary contribution from the Ministry of Education, Youth and Sports. Soon, we could again offer all our computational resources to our users.

Traditionally, my final words go to my colleagues standing behind IT4Innovations. Please check out our Review 2022 to find out that we have achieved a lot. With that in mind, I would like to thank everyone who has contributed to these achievements.



Vít Vondrák

Managing Director



↔ The IT4Innovations building was officially opened in 2014.

# 1

# IT4Innovations Profile

IT4Innovations National Supercomputing Center (IT4Innovations) is a university institute of VSB – Technical University of Ostrava, Czech Republic. It is a leading research, development, and innovation centre active in the fields of High-Performance Computing (HPC), Data Analysis (HPDA), Quantum Computing (QC), and Artificial Intelligence (AI) and their applications in other scientific fields, industry, and society. It operates the most powerful supercomputing systems in the Czech Republic. Together with the CESNET and CERIT-SC e-infrastructures, 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.

Since 2013, IT4Innovations has been providing state-of-the-art supercomputing technologies and services to both Czech and foreign research teams from academia and the private sector to increase the competitiveness and innovativeness of Czech science and industry.

IT4Innovations is currently operating three supercomputers: **Karolina** (15.7 PFlop/s, installed in the summer of 2021), **Barbora** (849 TFlop/s, installed in the autumn of 2019), and the specialised system for artificial intelligence computations **NVIDIA DGX-2** (2 PFlop/s for AI, installed in the spring of 2019). The Karolina supercomputer, procured within the EuroHPC Joint Undertaking and OP RDE Path to Exascale project. In the year of its installation, it was the most powerful supercomputer in the Czech Republic, ranked 69<sup>th</sup> in the TOP500 list of the world's most powerful supercomputers and 8<sup>th</sup> in the Green500 list of the most energy-efficient supercomputers. The very first supercomputers installed in IT4Innovations include Anselm

(94 TFlop/s, installed in the summer of 2013) and Salomon (2 PFlop/s, installed in the summer of 2015), and their operations were ceased in 2021.

Apart from the supercomputers operated at IT4Innovations, Czech research communities have had access to the **LUMI** supercomputer since the end of 2021, thanks to IT4Innovations' membership in the eponymous consortium. Located in the Finnish town of Kajaani, LUMI is the most powerful European supercomputer with a theoretical peak performance of 428 PFlop/s. IT4Innovations also participates in its operation.

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

#### **IT4Innovations' research activities are executed across five laboratories:**

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

IT4Innovations is currently the National Competence Centre in HPC, a member of the MaX and SPACE Centres of Excellence, and a partner in more than ten other international Horizon 2020 and Horizon Europe projects, coordinating the EXA4MIND project.

IT4Innovations has been highly active in collaboration with industry. In 2022, the European Digital Innovation Hub Ostrava (EDIH Ostrava) was established by combining the activities of IT4Innovations, the Faculty of Electrical Engineering and Informatics, which are part of VSB – Technical University Ostrava (VSB-TUO), and the Moravian-Silesian Innovation Centre Ostrava. EDIH Ostrava is part of the network of European Digital Innovation Hubs, which support the introduction and use of digital technologies primarily in small and medium-sized companies in order to support their competitiveness. The eponymous Digital Europe programme project supported the EDIH Ostrava foundation.

IT4Innovations is focused not only on providing access to state-of-the-art supercomputing systems and on activities in science and research but also on organising **a wide range of educational activities** focused on HPC, HPDA, AI, QC, and acquiring the knowledge to use the supercomputing infrastructure effectively. In the above fields, IT4Innovations is also involved in educating the next generation of experts, primarily within the **Computational and Applied Mathematics** MSc study programme and the **Informatics and Computational Science** PhD study programme. These programmes are jointly guaranteed with the Faculty of Electrical Engineering and Computer Science at VSB-TUO. Moreover, the centre's employees ensure 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, computer science, nanotechnology, and applied mechanics. In the autumn of 2022, the first pan-European Master's study programme focused on high-performance computing, **EUMaster4HPC**, was launched under the auspices of major European universities from the international project consortium of the same name, of which IT4Innovations is a member.

# History

- **2011** → Foundation of IT4Innovations → 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 • **2016** → Membership in ETP4HPC (European Technology Platform for High-Performance Computing) • **2018** → The Czech Republic joins the EuroHPC JU, in which IT4Innovations is actively involved → IT4Innovations becomes part of the H2020 POP2 Centre of Excellence and is registered by the European Commission as a Digital Innovation Hub • **2019** → Launching of the Bar-bora supercomputer, and the specialised NVIDIA DGX-2 system → Membership in BDVA (Big Data Value Association), and EUDAT CDI (EUDAT Collaborative Data Infrastructure) → Foundation of e-INFRA CZ → Launching of the H2020 LEXIS project, the coordinator of which was IT4Innovations
- **2020** → Foundation of the Digital Innovation Hub Ostrava → IT4Innovations becomes the National Competence Centre in HPC • **2021** → Launching of the Karolina supercomputer → Termination of operation of the Anselm, and Salomon supercomputers → Membership in the EOSC Association
- **2022** → Foundation of the European Digital Innovation Hub Ostrava (EDIH Ostrava) → LUMI-Q consortium's project to place a quantum computer at IT4Innovations approved

# Mission, Vision, and Memberships

## Mission

IT4Innovations' mission is to conduct excellent research in high-performance computing and advanced data analysis and to operate the leading national supercomputing infrastructure, strengthening its effective use to increase the competitiveness and innovation of Czech science and industry.

## Vision

IT4Innovations' vision is to become a leading supercomputing centre that provides professional services and conducts excellent research in high-performance computing and the processing of advanced data sets for the benefit of science, industry, and society.

## Membership

IT4Innovations actively participates in the EuroHPC Joint Undertaking activities and is a member of critical European infrastructures, initiatives, and associations in HPC and HPDA. They include the following:

- BDVA – Big Data Value Association
- EOSC – European Open Science Cloud
- ETP4HPC – European Technology Platform for High-Performance Computing
- EUDAT CDI – EUDAT Collaborative Data Infrastructure
- LUMI – Large Unified Modern Infrastructure
- PRACE – Partnership for Advanced Computing in Europe

# Organisational Structure

Scientific Council of IT4Innovations

Chairman | Doc. Vít Vondrák

Organisational Structure of IT4Innovations

Scientific Council | Managing Director | Doc. Vít Vondrák



## Internal Members

- Prof. Tomáš Kozubek
- Dr Branislav Jansík
- Dr Jan Martinovič
- Doc. Lubomír Říha
- Dr Tomáš Karásek
- Prof. Michal Otyepka
- Prof. Miroslav Vozňák

## External Members

- Prof. Jiří Damborský | Loschmidt laboratories of Masaryk University Brno
- Doc. Jiří Jaroš | Faculty of Information Technology, Brno University of Technology
- Dr Jakub Šístek | Institute of Mathematics of the Czech Academy of Sciences
- Doc. Pavel Jelínek | Institute of Physics of the Czech Academy of Sciences
- Prof. Jaroslav Pokorný | Faculty of Mathematics and Physics, Charles University

Employees of IT4Innovations

In 2022, the number of employees of IT4Innovations by divisions in full-time equivalent (FTE) was 148.14 FTE in total, which consists of:

**22%** Management and Administration

**14%** Supercomputing Services

**64%** Research and Development

- 43% Advanced Data Analysis and Simulations Lab
- 20% Modelling for Nanotechnologies Lab
- 17% Parallel Algorithms Research Lab
- 16% Infrastructure Research Lab
- 4% Big Data Analysis Lab



KAROLINA

KAROLINA

THE TECHNICAL FACILITY FOR NATIONAL SUPERCOMPUTING CENTER

EUROPEAN UNION  
Project Decision and Investment from the European Union

ERDF  
ERDF

Co-funded by the European Union

Project Partner Enterprise

↔ The Karolina supercomputer was made available to users of the computing infrastructure in August 2021.

# 2

## Important events in 2022

### JANUARY

- IT4Innovations joined the **EUPEX** (EUropean Pilot for EXascale) project to develop a prototype European exascale supercomputing platform, including a software stack and selected HPC applications.
- The H2020 **EUMaster4HPC** (European Master for High Performance Computing) project kicked off. It aims to create and subsequently implement the first pan-European Master's study programme focused on HPC.
- Scientists from several Czech research institutes, including IT4Innovations, developed **a new anode for lithium-ion batteries** based on graphitic acid - a densely carboxylated graphene derivative. The prestigious Advanced Energy Materials energy research journal published the research results.

### FEBRUARY

- Lukáš Halagačka from IT4Innovations has been conducting his studies of the structures of silicon nanowires for the preparation of solar cells at the prestigious École Polytechnique in Palaiseau since February.

### MARCH

→ The international [PRACE Summer of HPC 2021 Ambassador Award](#) went to Jenay Patel and Carola Ciaramelletti for their work on a project mentored by scientists from IT4Innovations.

→ IT4Innovations users have full access to the PROJECT data storage with a capacity of 15 PB.

### APRIL

→ The IT4Innovations seminar room was modernised to accommodate 37 people and is equipped with the latest audio-visual technology.

### MAY

→ The 5<sup>th</sup> [HPCSE](#) (The High Performance Computing in Science and Engineering) conference was held and organised by IT4Innovations.

→ The LUMI supercomputer ranked 3<sup>rd</sup> among the world's most powerful supercomputers in the TOP500 list.

→ LUMI also became the European number one in terms of energy efficiency. Thanks to the IT4Innovations membership in the LUMI consortium, its computational resources are also available to the Czech academic community.

### JUNE

→ Europe's top research infrastructures, including IT4Innovations, joined forces in the newly launched [BioDT](#) project (Biodiversity Digital Twin for Advanced Modelling, Simulation and Prediction Capabilities), funded by Horizon Europe, to jointly design and develop prototypes of digital twins for biodiversity research and analysis to support the EU Biodiversity Strategy 2030.

→ [The LUMI supercomputer inauguration ceremony](#) was held. In addition to the pan-European EuroHPC Joint Undertaking, the LUMI consortium countries, including the Czech Republic, also contributed to the funding.

### JULY

→ IT4Innovations hosted the ambassadors sitting on the [Committee of Permanent Representatives of the Member States to the Council of the EU](#).

→ IT4Innovations co-organised the [International Conference on Domain Decomposition Methods \(DD27\)](#) in Prague, bringing together world leaders in the field that combines numerical mathematics with the world of powerful supercomputers.

### SEPTEMBER

→ The Horizon Europe [OpenWebSearch.EU](#) project coordinated by the Universität Passau, Germany, was launched. The project aims to create an open European web search infrastructure.

→ IT4Innovations researchers organised the [hackathon to develop the FIJI software](#) for bioimage processing.

→ A new, recyclable [material capable of detecting and eradicating heavy metals](#) was developed by IT4Innovations researchers in collaboration with scientists from several research centres. The research results were published in the Small Journal.

→ The [Researcher's Night](#) event attracted a record 900 visitors to IT4Innovations.

## OCTOBER

→ Professor [Pavel Hobza](#), a Modelling for Nanotechnologies Lab member, won the [Neuron Endowment Fund Prize](#) in chemistry.

→ Georg Zitzlsberger obtained two NVIDIA Deep Learning Institute certificates for AI – Applications of AI for Anomaly Detection and Applications of AI for Predictive Maintenance.

→ Kristian Kadlubiak successfully completed the Train the Trainer certification programme on parallel programming under the auspices of the Höchstleistungsrechenzentrum Stuttgart (HLRS).

## NOVEMBER

→ The [European Digital Innovation Hub Ostrava](#) was founded by combining the activities of IT4Innovations, the Faculty of Electrical Engineering and Computer Science of VSB-TUO, and the Moravian-Silesian Innovation Centre Ostrava.

→ The 6<sup>th</sup> edition of the [IT4Innovations Users' Conference](#) took place. After two years of virtual meetings caused by the COVID-19 pandemic, it welcomed 80 guests this year.

→ Markéta Hrabánková, Ondřej Meca, Tomáš Brzobohatý, Lubomír Říha, Milan Jaroš, and Petr Strakoš received the [Best Research Poster Award](#) for their contribution entitled Toward Scalable Voxelization of Meshes with High Growth Rate at the SC22 Conference held in Dallas, Texas, USA.

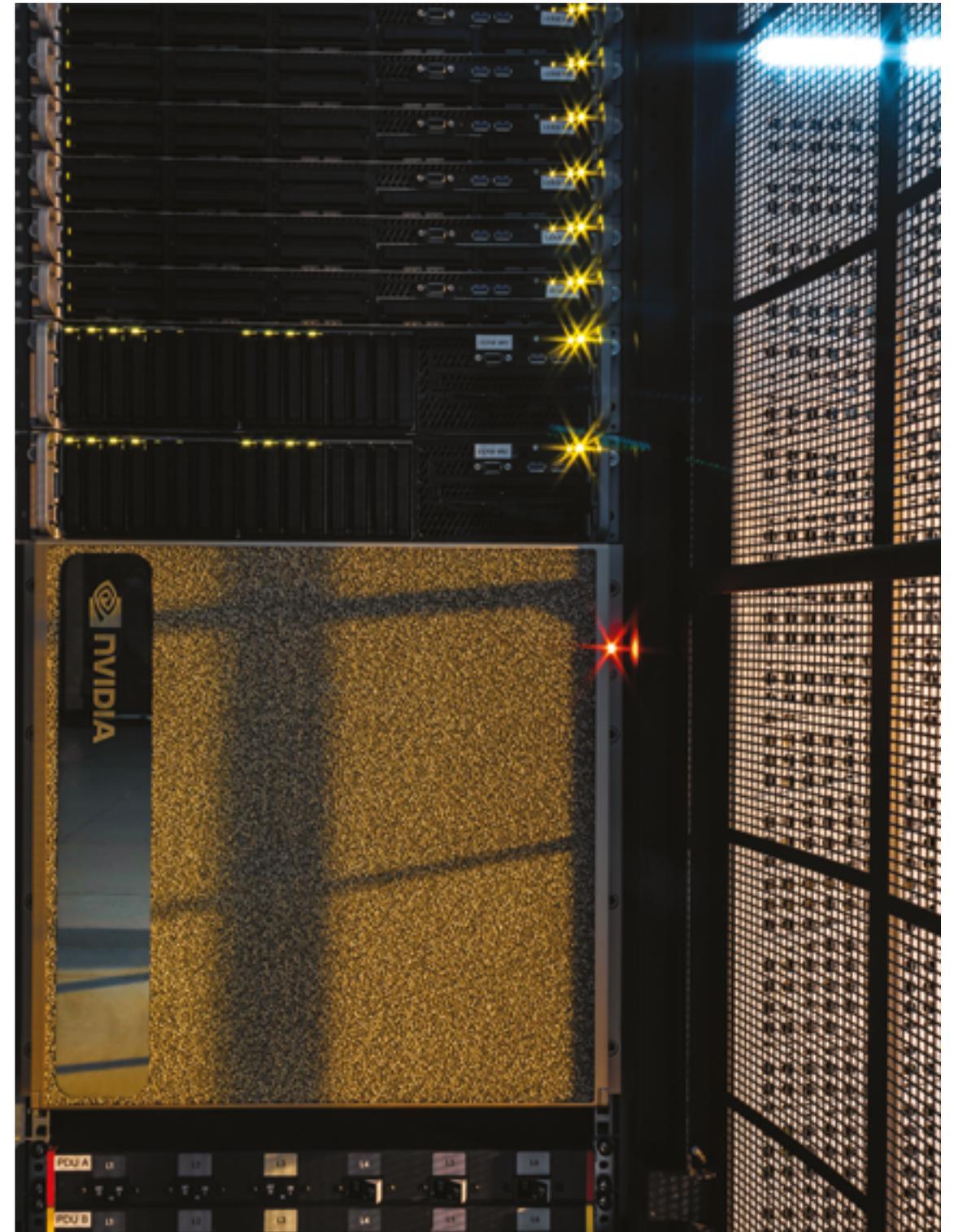
→ The [complementary systems](#) (Phase I) were put into operation. They are also embedded with new programming models, libraries, and application development tools that can derive maximum performance from this hardware.

→ IT4Innovations co-organised the [European Big Data Value Forum](#) (EBDVF) 2022 conference in Prague, where 400 guests meet.

## DECEMBER

→ IT4Innovations participated in developing and upgrading specialised software for easier and faster protein research as part of the [PerMed Centre](#) project. The software, made available free of charge to researchers, opens up new possibilities for drug design.

→ IT4Innovations collaborated with the [Police of the Czech Republic](#) and developed a tool to fight criminality more effectively.



↔ NVIDIA-DGX2

The NVIDIA DGX-2 system is designed to solve the most demanding AI tasks, achieving a peak performance of 2 PFlop/s. The system was installed at IT4Innovations in 2019.

# 3

## Financial Review

### IT4Innovations Economic Balance

The total expenditures of IT4Innovations amounted to **CZK 305,388,000**, 94.3% and 5.7% of which were operational (non-investment) and investment (capital) expenditures, respectively.

Operational expenditures amounted to CZK 288 million in 2022. The largest part of these expenditures consisted of salary expenses, overheads, and services (costs of electricity consumption, maintenance of the operated systems and supporting infrastructure, technical and system support, etc.).

The investment expenditures in 2022 amounted to CZK 17.3 million, including the acquisition of the complementary systems - Phase I, electricity metering in the data room and the modernisation of the seminar room.

**Profit before tax amounted to CZK 7,154,000.**

## Economic balance of IT4Innovations

Personnel costs – research labs	CZK 83,768,000
Overheads	CZK 64,401,000
Services	CZK 62,923,000
Personnel costs – management, administration	CZK 37,587,000
Personnel costs – supercomputing services	CZK 20,325,000
International and domestic business trips	CZK 9,163,000
Small fixed assets	CZK 4,223,000
Scholarships	CZK 1,920,000
Fees	CZK 1,897,000
Consumables	CZK 1,610,000
Other costs	CZK 245,000
<b>A. Total operational expenditures</b>	<b>CZK 288,062,000</b>
Tangible fixed assets – machines and equipment	CZK 14,481,000
Tangible fixed assets – buildings	CZK 1,579,000
Intangible fixed assets	CZK 1,266,000
<b>B. Total investment expenditure</b>	<b>CZK 17,326,000</b>
<b>C. Total expenditures (A+B)</b>	<b>CZK 305,388,000</b>
<b>D. Total sources of funding</b>	<b>CZK 312,542,000</b>
<b>E. Balance total (D-C)</b>	<b>CZK 7,154,000</b>

## Sources of Funding

In 2022, the overall budget of IT4Innovations was CZK 312,542,000. National grants accounted for the largest share of the funding sources, followed by structural funds. The third most important source of funding for IT4Innovations was international projects.

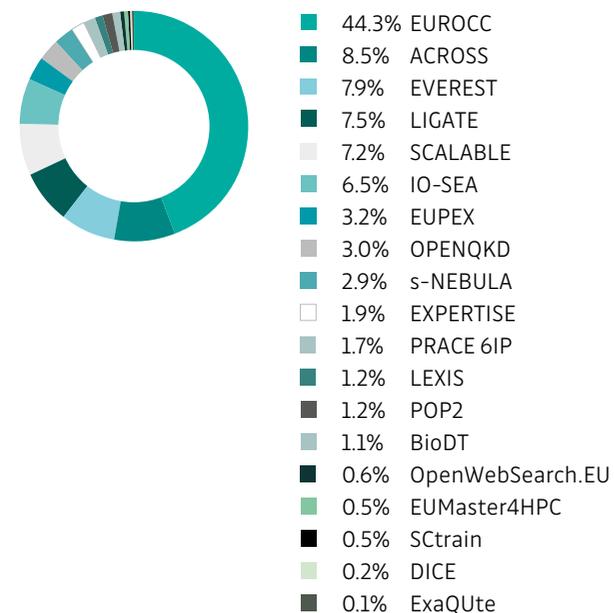
## Sources of funding for the Institute's costs

CZK 312,542,000 in total



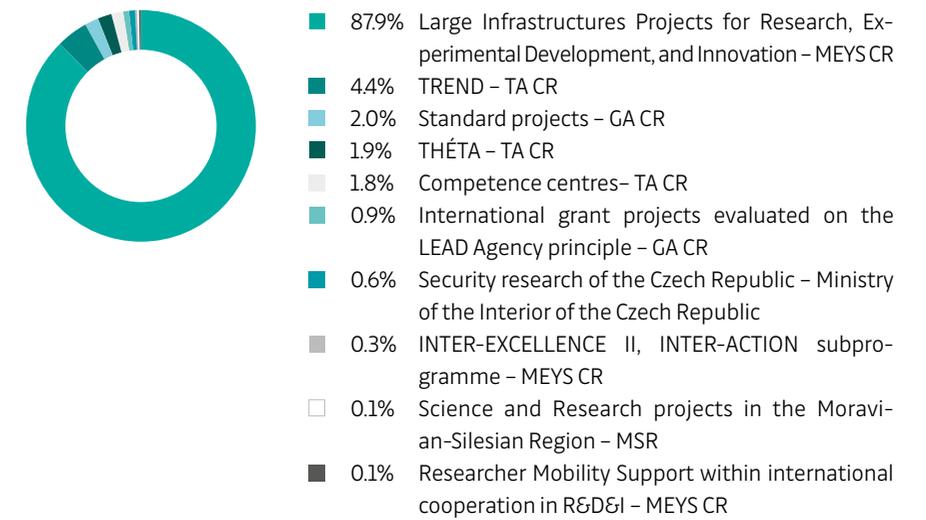
## International projects

CZK 55,039,000 in total



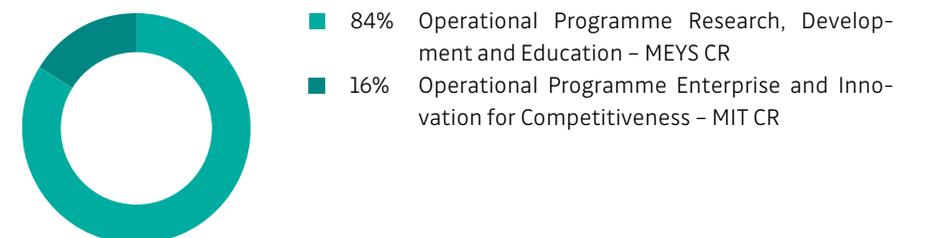
## National projects

CZK 130,437,000 in total



## Structural funds

CZK 61,466,000 in total



# List of IT4Innovations Projects

## National Grants

### Projects supported by the Ministry of Education, Youth and Sports (MEYS CR)

Large Infrastructure for Research, Experimental Development and Innovation Project

→ e-Infrastructure CZ

Projects of the Operational Programme Research, Development and Education

→ IT4Innovations National Supercomputing Center – Path to Exascale

→ e-INFRA CZ: Modernisation

→ Artificial Intelligence and Reasoning

→ Modelling of Collision Processes in Low-Temperature Plasma

→ Development of a tool for scientific data processing and visualisation in VR with multi-user support

→ Novel sources of THz radiation based on spintronic effects

→ Development of Computational Algorithms for Solution of Nonlinear Structural Dynamical Problems with Utilisation of ESPRESO Numerical Library

→ Doctoral School for Education in Mathematical Methods and Tools in HPC

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

→ Multiscale design of novel Rare Earth free permanent magnets

International cooperation in Research and Development

→ Influence of thermoelectrical effects on spin-orbit torques in 2D van der Waals materials

### Projects supported by the Moravian-Silesian Region (MSR)

Individual projects

→ Digital Innovation Hub – Pilot Verification

### Projects supported by the Grant Agency of the Czech Republic (GA CR)

International Grant Projects Evaluated by the LEAD Agency

→ Magnetism at interfaces: from quantum to reality

Standard Grant Projects

→ Tailoring thermal stability of W-Cr based alloys for fusion application

→ Unconventional superconductors under extreme conditions

### Projects supported by the Technology Agency of the Czech Republic (TA CR)

National Competence Centres Programme

→ Personalised Medicine – Diagnostics and Therapy

TREND Programme

→ 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

ÉTA Programme

→ Creating a model for evaluating the impact of changes in the parameters of the tax-benefit system on the socio-economic situation of families with children in the Czech Republic

### Projects supported by the Ministry of Industry and Trade (MIT CR)

Operational Programme Enterprise and Innovation for Competitiveness

→ Digital twin of product within Siemens plants

→ SmartFleet – AI based software for a full utilisation of electric cars in companies and maximisation of their share in the car fleet

→ Holograms with active security elements

→ Research and development of application SW tool for effective evaluation of catalytic processes

→ Development, security, and scalability of cloud services in the area of digital transformation

### VSĚ-TUO Projects with IT4Innovations participation

→ Projects of talented VSĚ-TUO PhD students (projects supported by the MSR)

→ Technology for the Future 2.0 (project supported by MEYS CR)

→ Science without borders 2.0 (project supported by MEYS CR)

→ Employment of artificial intelligence into an emergency call reception (project supported by MIT CR)

→ National Centre for Energy (NCE), (project supported by TA CR)

→ Energy System for Grids (project supported by TA CR)

→ CEET – Centre for Energy and Environmental Technologies (project supported by TA CR)

→ Common Actuator Controller (project supported by MIT CR)

## International Grants

### Projects of the 8<sup>th</sup> Framework Programme for Research and Innovations of the European Union – Horizon 2020

→ EUROCC – National Competence Centres in the framework of EuroHPC

→ PRACE-6IP – Partnership for Advanced Computing in Europe, 6<sup>th</sup> Implementation Phase

→ POP2 – Performance Optimisation and Productivity 2

→ LIGATE – Ligand Generator and portable drug discovery platform AT Exascale

→ EVEREST – dEsign enVironmEnt foR Extreme-Scale big data analyTics on heterogeneous platforms

→ ACROSS – HPC big dAta artiFiCial intelligence cross stack platfoRm tOwardS exaScale

→ s-NEBULA – Novel Spin-Based Building Blocks for Advanced TeraHertz Applications

→ SCALABLE – SCALable LAttice Boltzmann Leaps to Exascale

→ IO-SEA – IO Software for Exascale Architecture

→ OPENQKD – Open European Quantum Key Distribution Testbed

→ DICE – Data Infrastructure Capacity for EOSC

→ EUPEX – European Pilot for Exascale

→ EUMaster4HPC – European Master for High-Performance Computing

### Projects of the 9<sup>th</sup> Framework Programme for Research and Innovations of the European Union – Horizon Europe

→ BioDT – Biodiversity Digital Twin for Advanced Modelling, Simulation and Prediction Capabilities

→ OpenWebSearch.EU

### Erasmus+ projects

→ SCtrain – Supercomputing knowledge partnership

# 4

## Supercomputing Services

IT4Innovations operates the most powerful supercomputing systems in the Czech Republic, primarily used by academia and research and development organisations. Part of the capacity is dedicated to developing collaboration between academia and industry and for contract partners in the form of commercial rental.

In 2022, IT4Innovations operated three supercomputers – **Karolina** (15.7 PFlop/s), **Barbora** (849 TFlop/s), and the **NVIDIA DGX-2** specialised system for artificial intelligence calculations (130 TFlop/s and 2 PFlop/s for AI).

The petascale Karolina system was made fully operational in the summer of 2021. It was acquired as part of the pan-European EuroHPC Joint Undertaking, with 35% of its computational resources available to users from EuroHPC membership countries. Immediately after its launch, it ranked among the most powerful HPC systems in Europe – in the TOP500 list, which evaluates supercomputers in terms of their performance, it ranked 69<sup>th</sup> worldwide, 19<sup>th</sup> in Europe, and in the Green500 list of the most energy-efficient supercomputers, it ranked 8<sup>th</sup> globally and 3<sup>rd</sup> in Europe.

In 2022, the **LUMI** supercomputer, with its theoretical peak performance reaching 428 PFlop/s, was also fully commissioned. Thanks to IT4Innovations' membership in the LUMI (Large Unified Modern Infrastructure) consortium consisting of ten European countries, Czech scientists can compute on one of the world's most powerful and advanced supercomputers. IT4Innovations participates in the implementation of this project as part of its management structure, provides expert support to users within the so-called LUST (LUMI user support team), and develops software tools

such as HyperQueue, which enable users to use the available computational resources of LUMI effectively.

The latest addition to IT4Innovations is **complementary systems** (Phase I), consisting of several hardware platforms. These systems provide access to emerging, non-traditional, and highly specialised hardware architectures that are not yet common in supercomputing centres. The first part was put into operation in IT4Innovations in the autumn of 2022 and includes models, libraries, and tools for application development. Additional hardware platforms will be delivered in 2023.

Apart from supercomputers, the IT4Innovations data room also houses **large-capacity PROJECT data storage**, which are used for storing and backing up data processed or generated on the Ostrava supercomputers.



↔ IT4Innovations Data Room

# Technical Specifications of the Supercomputers

	Barbora	Karolina	NVIDIA DGX-2	LUMI
Put into operation	autumn 2019	summer 2021	spring 2019	autumn 2022
Theoretical peak performance	849 TFlop/s	15.7 PFlop/s	130 TFlop/s, 2 PFlop/s for AI	428.7 PFlop/s
Operating system	CentOS 64bit 7.x	Centos 64 bit 7.x	CentOS 64bit 7.x	Custom Cray
Compute nodes	201	831	1	4,096
CPU	2x Intel Cascade Lake, 18 cores, 2.6 GHz, 7,236 cores in total	720x 2x AMD 7H12, 64 cores, 2.6 GHz, 92,160 cores in total 72x 2x AMD 7763, 64 cores, 2.45 GHz, 9,216 cores in total 72x 8x NVIDIA A100 GPU, 576 GPU in total 32x Intel Xeon-SC 8628, 24 cores, 2.9 GHz, 768 cores in total 36x 2x AMD 7H12, 64 cores, 2.6 GHz, 4,608 cores in total 2x 2x AMD 7452, 32 cores, 2.35 GHz, 128 cores in total	2x Intel Xeon Platinum, 24 cores, 48 cores in total	1,376x AMD EPYC 7763, 2.45/3.5 GHz, 128 cores (2x64), 176,128 cores in total 128x AMD EPYC 7763, 2.45/3.5 GHz, 128 cores (2x64), 16,384 cores in total 32x AMD EPYC 7763, 2.45/3.5 GHz, 128 cores (2x64), 8,192 cores in total 2,560x AMD EPYC 7A53, 2.45/3.5 GHz, 128 cores (2x64), 327,680 cores in total 10,240x AMD Instinct MI250X GPUs, 14,080 stream processors per GPU
RAM per compute node	192 GB 6 TB fat node	256 GB / 1 TB (GPU) / 24 TB fat node 320 GB HBM2 (8 x 40 GB) GPU	1.5 TB DDR4, 512 GB HBM2 (16 x 32 GB)	256 GB / 512 GB / 1,024 GB
GPU accelerators	32x NVIDIA Tesla V100	576x NVIDIA A100	16x NVIDIA Tesla V100 32 GB HBM2	N/A
Storage	29 TB / home, 310 TB / scratch (28 GB/s)	30.6 TB / home (1.93 GB/s sequential write performance, 3.10 GB/s sequential read performance), 1,361 TB / scratch (NVMe, 730.9 GB/s sequential write performance, 1,198.3 GB/s sequential read performance)	30 TB NVMe	80 PB ( /home + /project + /scratch ) 240 GB/s
Interconnection	Infiniband HDR 200 Gb/s	Infiniband HDR 200 Gb/s	8 x Infiniband nebo 8 x 100 GbE	200 Gb/s Slingshot-11



↔ In 2022, IT4Innovations operated three supercomputers, Barbora, NVIDIA-DGX2 and Karolina.

# Computational Resource Allocations

Providing computational resources is one of the primary missions of IT4Innovations. Supercomputers have been continuously available to the Czech scientific community and industrial companies since 2013, when the Anselm supercomputer was launched.

As of 2022, IT4Innovations has changed the unit of computational resources allocation from core hours to node hours, reflecting the different computing architecture of the clusters, e.g., CPU and GPU. Applicants must specify in their project requests which nodes of which cluster they want to use in what quantities to solve scientific problems (Barbora CPU, Barbora GPU, Barbora FAT, DGX-2, Karolina CPU, Karolina GPU, Karolina FAT, LUMI CPU, LUMI GPU).

From 2013 to the end of 2022, [1,719 projects](#) in various scientific fields, such as new materials and drug design, physics laws discovery, engineering problems, rendering, and scientific data visualisation, to projects addressing cybersecurity, advanced data analytics, and AI tasks, have received computational resources.

The demand for computational resources is higher year by year, and each new Open Access Grant Competition announced confirms that the scientific community in the Czech Republic relies on powerful supercomputers and builds its scientific work on them.

The computational resources of IT4Innovations supercomputers can be obtained in one of the following ways:

- a) The largest share of the computational resources is distributed within the [Open Access Grant Competitions](#) framework, which IT4Innovations announces three times a year. They are open to researchers and academics from the Czech Republic. Submitted projects are subject to the approval of the allocation committee based on an expert evaluation of scientific excellence, computational readiness, and socio-economic impact.
- b) [Director's discretion](#) – applications are submitted continuously and only in cases where Open Access Grant Competitions cannot be used. This is an irregular allocation of computational resources approved by IT4Innovations management.
- c) [Rental of computational resources](#) – This is paid access to the computational resources of the supercomputers operated, which is charged at market rates according to the current IT4Innovations tariff.
- d) Access to Ostrava's computing infrastructure can also be obtained through [European grant competitions](#) announced by the EuroHPC Joint Undertaking.

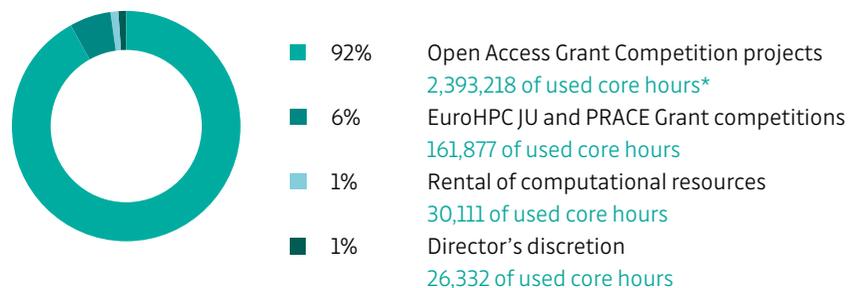


↔ [Barbora](#)

The Barbora supercomputer was put into operation in 2019 as part of the modernisation of the computing infrastructure. As well as other Ostrava supercomputers, the name Barbora came from a survey involving the general public.

The number of active projects was 260 in 2022. The computational resources these projects were awarded amounted to a total of **2,611,538 node hours**.

### Distribution of computational resources in 2022



\* The used node hours give an idea of how many computational resources were used in 2022. The total value here consists of all projects calculated at IT4Innovations that year.

### Open Access Grant Competitions – 24<sup>th</sup>, 25<sup>th</sup>, 26<sup>th</sup> call

In 2022, three Open Access Grant Competitions and two Special Calls were announced, supporting **186 research projects**, 14 of which were multi-year ones. Specifically, these were the 24<sup>th</sup>, 25<sup>th</sup> and 26<sup>th</sup> calls and two special calls for the 24<sup>th</sup> and 26<sup>th</sup> Open Access Grant Competitions. According to the schedule of each call, successful applicants were granted access to computational resources during 2022. For standard projects, computational resources are provided for nine months; for multi-year projects, for 18, 27, or 36 months, and they are intended to support long-term research grants.

In these three Open Access Grant Competitions (and two special calls), users applied for a total of 5.92 million node hours. Given the high demand for computational resources exceeding the resources offered, the Allocation Committee decided to reduce the allocations of the evaluated projects. The reduction affected all projects proportionally. In total, 5.7 million node hours were allocated to projects in these calls of the Open Access Grant Competition. Some projects were also allocated computational resources of the LUMI supercomputer.

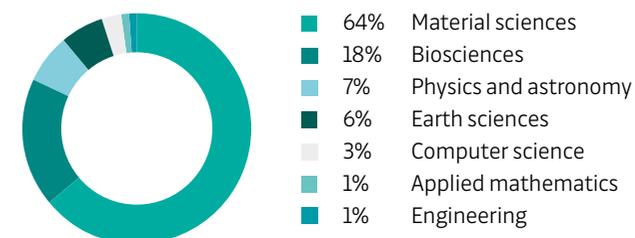
Projects in the field of material sciences received the most computational resources, accounting for 64%. Life sciences projects came in second place with 18% and physics and astronomy projects came in third with 7%.

By institution, scientists from VSB-TUO and investigators from the Czech Academy of Sciences used the most computational resources of the IT4Innovations supercomputers, followed by CEITEC and Charles University.

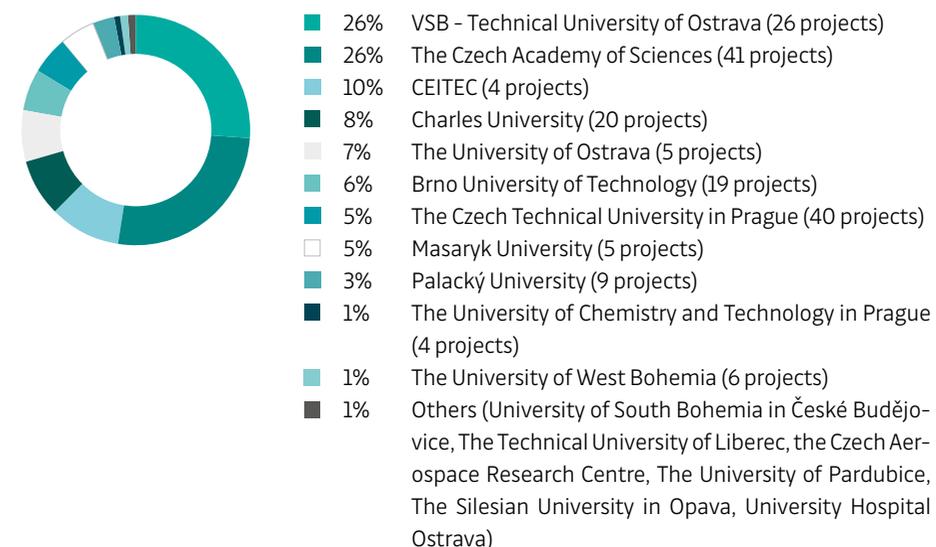
Most of the projects that received computational resources were submitted by scientists from institutes of the Czech Academy of Sciences (41 projects in total), Czech Technical University in Prague (40 projects), and VSB-TUO (26 projects).

Investigators from 13 different institutes of the Czech Academy of Sciences received computational resources for their projects, with the institutes using the IT4Innovations infrastructure, the most being the Institute of Organic Chemistry and Biochemistry, the Institute of Computer Science, the Institute of Physics of Materials, the Institute of Physics, and the J. Heyrovský Institute of Physical Chemistry.

### Computational resources allocated within the Open Access Grant Competitions in 2022 by scientific discipline



### Computational resources allocated within the Open Access Grant Competitions in 2022 by institutions



### Director's discretion

In 2022, 15 projects using more than 26 thousand node hours were supported within the Director's discretion scheme.

### Rental of computational resources

The computational resources used within the paid rental scheme amounted to 30 thousand node hours in 2022. These were commercial projects of the following companies: Sotio a.s., DHI a.s., LightOn SAS, and Varroc Lighting Systems, s.r.o.

### EuroHPC JU and PRACE grant competitions

In 2022, nearly 162 thousand node hours were used within these competitions, shared by 27 projects. Of these, 25 and 2 projects were carried out under the EuroHPC JU and PRACE calls, respectively.

### Users of computational resources

The number of active users of the IT4Innovations computing infrastructure increased by 63% year-on-year to 1,408 in 2022.

The IT4Innovations Technical Support provided to its users received a total of 1,275 queries and requests. The internal response time (24 hours for the first response) was met for 99.9% of the queries. The internal closure time, which should not exceed 30 days, was met for 95.3% of the queries.

# 5

## Research and Development

IT4Innovations conduct excellent research in the fields of high-performance computing (HPC), data analysis (HPDA), quantum computing (QC), and artificial intelligence (AI), including their applications in science and industry. The key research areas of IT4Innovations include big data processing and analysis, machine learning, quantum computing, development of parallel scalable algorithms, solving computationally demanding engineering problems, advanced visualisation, virtual reality, modelling for nanotechnologies, and material design.

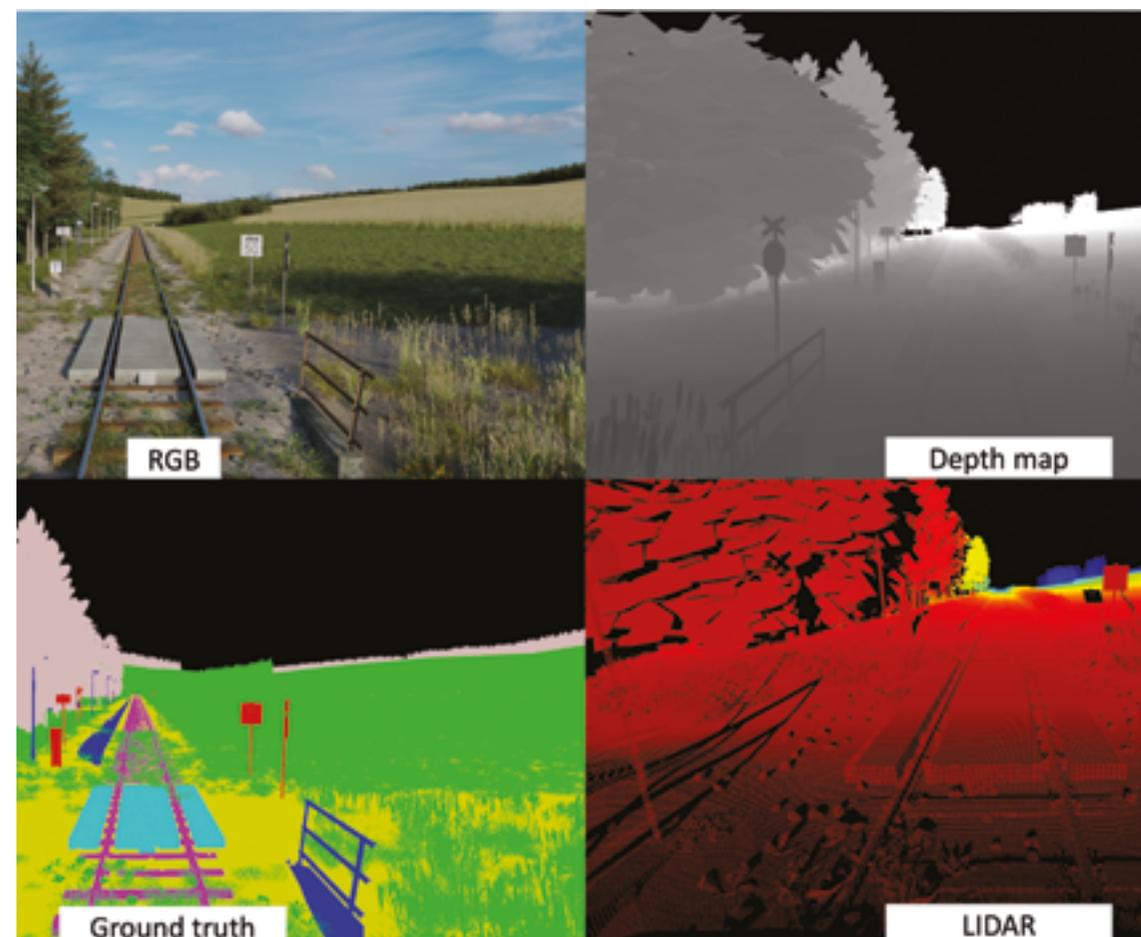
IT4Innovations is a research and development centre with strong international links, and as such, it actively participates in all activities of the EuroHPC Joint Undertaking and in several prestigious international organisations (PRACE, ETP4HPC, EUDAT, BDVA, EOSC). In 2022, it participated in implementing 15 international projects funded by Horizon 2020 and Horizon Europe and was a member of the H2020 POP2 Centre of Excellence.

IT4Innovations has been the National Centre of Competence for HPC within the European EuroCC project since 2020. Moreover, IT4Innovations is involved in developing the Urban Thematic Exploitation Platform funded by the European Space Agency (ESA) and the ESA BLENDED (Blockchain ENabled DEep Learning for Space Data) project. In the past, IT4Innovations participated in some 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 carried out across five laboratories:

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

In 2022, IT4Innovations research labs were awarded nearly 1.2 million node hours within Open Access Grant Competitions, representing 20% of the total allocation of all supported projects. Most of the projects and the computational resources were awarded to the Modelling for Nanotechnologies Lab.



↔ Simulator of train track conditions to improve obstacle detection in real traffic

In cooperation with the IXPERTA s.r.o. company, a functional sample of a railway vehicle detecting obstacles in the driving profile was developed.

# Research and Development Flagships

In 2022, 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.

ESPRESO, Highly Parallel Finite Element Package for Engineering Simulations

**Principal Investigators:** Dr Tomáš Brzobohatý, Dr Ondřej Meca, Doc. Lubomír Říha  
The solver was refactored to use the ARM architecture as part of the team's research activities involved in developing the open-source ESPRESO tool. Along with this task, carried out within the European EUPEX project, the physical matrix builder was modularly redesigned to efficiently use the vectorised instructions available on modern processors such as the AVX512 and SVE. Testing was also carried out on Intel's Ponte Vecchio accelerators, which are expected to be available by the end of 2023. The ESPRESO library also includes MESIO, a highly parallel postprocessing tool for converting numerical simulation results from both ESPRESO itself and third-party packages into a hierarchical structure, allowing the connection of professional 3D visualisation tools. This connection enables, for example, the efficient display of detailed simulations in the form of volumetric renderings processed using a professional path-tracing renderer in combination with the freely available BLENDER tool. Research in this area has been recognised at a major HPC event in 2022, the SC22 conference in Dallas, USA.

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 vital 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) the verification of experiments, ii) simulating conditions or calculating material properties that are not directly accessible or measurable, and iii) designing novel materials. Within the flagship, we covered essential and cutting-edge topics to maximise or minimise the heat transfer between materials. The former is used to design more efficient nuclear fuel materials from radioactive compounds for Generation IV nuclear reactors. The latter to optimise the thermoelectric phenomenon, materials for converting heat to electricity under normal conditions. Furthermore, these calculations allow us to model magnetostrictive and magneto-elastic properties, i.e., for alloys where it is desirable to suppress natural thermal expansion, actuators, and ultra-precision sensors used in nano-robotics, aerospace, and aeronautics.

HPC platforms for scientific workflow execution

**Principal Investigators:** Dr Jan Martinovič, Dr Ada Böhm, Dr Václav Svatoň

The main goal of most supercomputing centres is to lower the entry barriers to the world of high-performance computing for all users from research institutes, industry, hospitals, state administration, etc., while not sacrificing execution performance. The flagship team is focused on developing the HPC-as-a-Service (HaaS) concept. It is an integral solution for HPC centres to make their 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. Still, it aims to provide a solution that 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 the HPC workloads are scientific pipelines created by domain specialists who need deep knowledge of HPC technologies. The team continued to develop programming models capable of a user-friendly workload description and runtime layers capable of efficient execution in large-scale distributed environments (e.g., in-house HyperTools toolset). Finally, the aim is also to make the results accessible and thus maximise their potential impact.



↔ Numerical simulations

IT4Innovations develops a simulation tool for solving complex engineering problems such as heat transfer, structural mechanics, vibration, and noise propagation.

# Summary of Science and Research Results in 2022

Science and research results in 2022 based on the RIV 2017+ Methodology

This subsection presents the results of IT4Innovations science and research in 2022.

## Summary of the achieved IT4Innovations science and research results in 2022

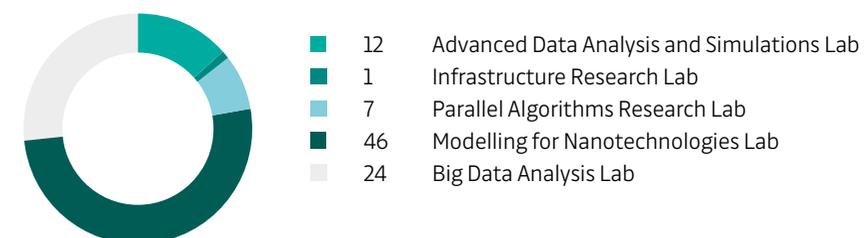
Results classified based on the RIV 2017+ Methodology	Achieved results
Jimp – article in the Web of Science database	84
JSC – article in the SCOPUS database	6
Jost – other reviewed articles	0
B – reviewed publication	2
C – chapter in a reviewed publication	7
D – section in a proceeding	29
P – patent	1
F – utility model, industrial design	1
Z – semioperation, verified technology	0
G – prototype, functional sample	4
H – results reflected in norms and directives	0
N – methodology, specialised map	0
R – software	17
V – research report	7

## Jimp and JSC Journal Publications in 2022 by individual labs and ranking

Publications by individual labs and ranking	D1	Q1/D1	Q2	Q3	Q4	Total
Advanced Data Analysis and Simulations Lab	5	7	0	0	0	12
Infrastructure Research Lab	0,5	0,5	0	0	0	1
Parallel Algorithms Research Lab	2,5	3,5	0	1	0	7
Modelling for Nanotechnologies Lab	22	19	5	0	0	46
Big Data Analysis Lab	11	4	7	1	1	24
Total	41	34	12	2	1	90

The division of journals into D1, Q1/D1, ..., and Q4 categories is determined by their best position in the scientific field categories in the Web of Science and Scopus.

## Number of journal publications in 2022 by individual labs



## List of D1 publications sorted by individual labs

### Advanced Data Analysis and Simulations Lab

- Lampart Marek, Lampartová Alžběta, Orlando Giuseppe: *On extensive dynamics of a Cournot heterogeneous model with optimal response*. CHAOS, 2022. DOI 10.1063/5.0082439, IF 3.741 (JIMP)
- Pinto Pedro; Bispo Joao, Cardoso Joao, Barbosa Jorge Gomes, Gadioli Davide, Palermo Gianluca, Martinovič Jan, Golasowski Martin, Slaninová Kateřina, Cmar Radim, Silvano Cristina: *Pegasus: Performance Engineering for Software Applications Targeting HPC Systems*. IEEE Transactions on Software Engineering, 2022. DOI 10.1109/TSE.2020.3001257, IF 9.322 (JIMP)
- Struhár Juraj, Rapant Petr, Kačmařík Michal, Hlaváčová Ivana, Lazecký Milan: *Monitoring Non-Linear Ground Motion above Underground Gas Storage Using GNSS and PSInSAR Based on Sentinel-1 Data*. Remote Sensing, 2022. DOI 10.3390/rs14194898, IF 5.349 (JIMP)
- Martinovič Tomáš, Fulneček Jan: *Fast Algorithm for Contactless Partial Discharge Detection on Remote Gateway Device*. IEEE Transactions on Power Delivery, 2022. DOI 10.1109/TPWRD.2021.3104746, IF 4.825 (JIMP)
- Smail Tayeb, Abed Mohamed, Mebarki Ahmed, Lazecký Milan: *Earthquake-induced landslide monitoring and survey by means of InSAR*. Natural Hazards and Earth System Sciences, 2022. DOI 10.5194/nhess-22-1609-2022, IF 4.58 (JIMP)

### Infrastructure Research Lab

- Meca Ondřej, Říha Lubomír, Jansík Branislav, Brzobohatý Tomáš: *Toward highly parallel loading of unstructured meshes*. Advances in Engineering Software, 2022. DOI 10.1016/j.advengsoft.2022.103100, IF 4.255 (JIMP)

### Parallel Algorithms Research Lab

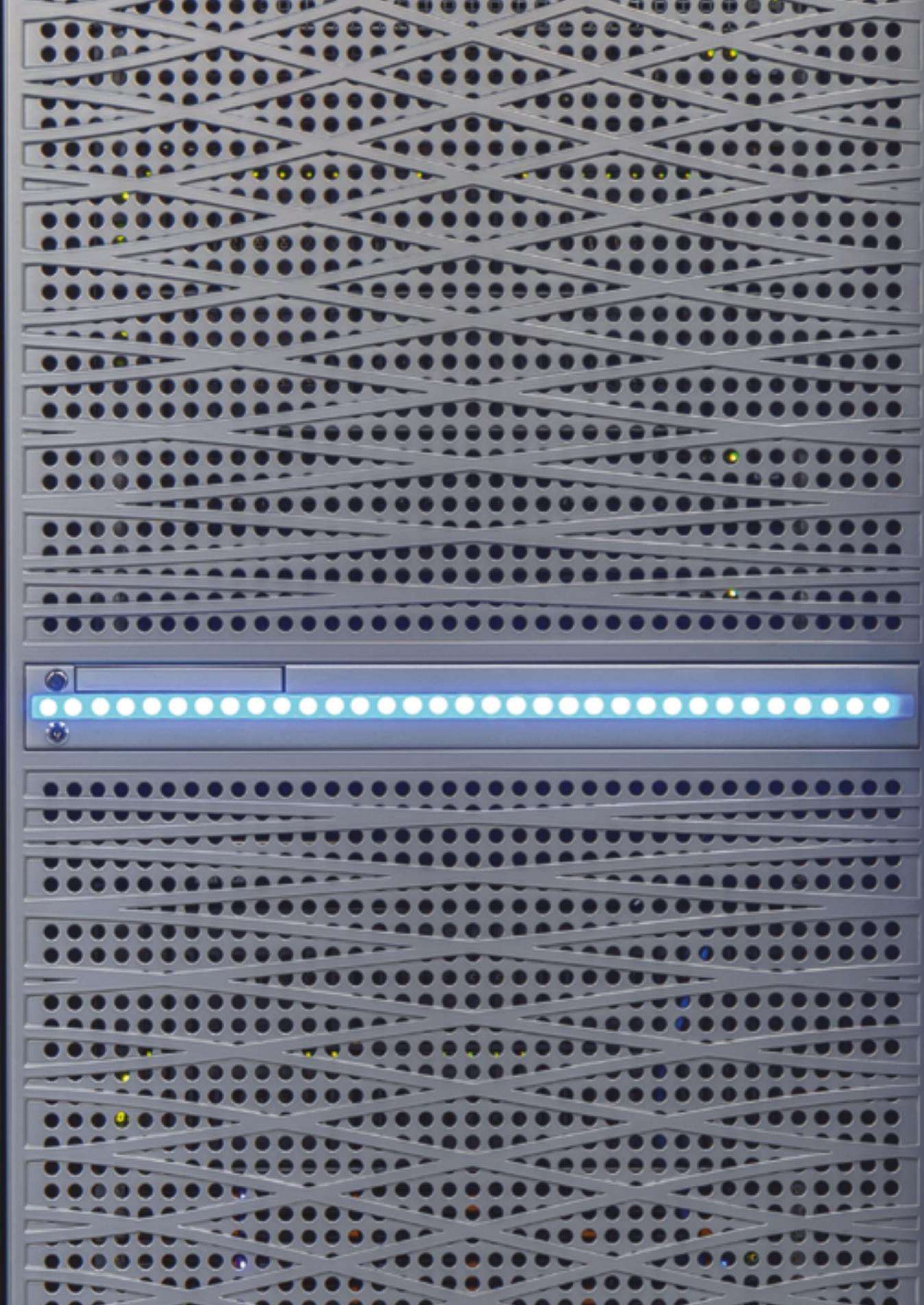
- Gebauer Marek, Blejchař Tomáš, Brzobohatý Tomáš, Karásek Tomáš, Nevřela Miroslav: *Determination of Aerodynamic Losses of Electric Motors*. Symmetry, 2022. DOI 10.3390/sym14112399, IF 2.94 (JIMP)

- Zapoměl Jaroslav, Ferfecki Petr: *A new concept of a hydrodynamic bearing lubricated by composite magnetic fluid for controlling the bearing load capacity*. Mechanical Systems and Signal Processing, 2022. DOI 10.1016/j.ymssp.2021.108678, IF 8.934 (JIMP)
- Meca Ondřej, Říha Lubomír, Jansík Branislav, Brzobohatý Tomáš: *Toward highly parallel loading of unstructured meshes*. Advances in Engineering Software, 2022. DOI 10.1016/j.advengsoft.2022.103100, IF 4.255 (JIMP)

### Modelling for Nanotechnologies Lab

- Sedajova Veronika, Bakandritsos Aristeidis, Blonski Piotr, Medved Miroslav, Langer Rostislav, Zaoralova Dagmar, Ugolotti Juri, Dzibelova Jana, Jakubec Petr, Kupka Vojtech, Otyepka Michal: *Nitrogen doped graphene with diamond-like bonds achieves unprecedented energy density at high power in a symmetric sustainable supercapacitor*. Energy & Environmental Science, 2022. DOI 10.1039/d1ee02234b, IF 39.714 (JIMP)
- Mlynsky Vojtech, Janecek Michal, Kuhrova Petra, Frohling Thorben, Otyepka Michal, Bussi Giovanni, Banas Pavel, Sponer Jiri: *Toward Convergence in Folding Simulations of RNA Tetraloops: Comparison of Enhanced Sampling Techniques and Effects of Force Field Modifications*. Journal of Chemical Theory and Computation, 2022. DOI 10.1021/acs.jctc.1c01222, IF 6.578 (JIMP)
- Pykal Martin, Vondrak Martin, Srejber Martin, Tantis Iosif, Mohammadi Elmira, Bakandritsos Aristeidis, Medved Miroslav, Otyepka Michal: *Accessibility of grafted functional groups limits reactivity of covalent graphene derivatives*. Applied Surface Science, 2022. DOI 10.1016/j.apsusc.2022.153792, IF 7.392 (JIMP)
- Kývala Lukáš, Havela L., Kadzielawa Andrzej Piotr, Legut Dominik: *Electrons and phonons in uranium hydrides - effects of polar bonding*. Journal of Nuclear Materials, 2022. DOI 10.1016/j.jnucmat.2022.153817, IF 3.555 (JIMP)
- Hruby Vitezslav, Zdrzil Lukas, Dzibelova Jana, Sedajova Veronika, Bakandritsos Aristeidis, Lazar Petr, Otyepka Michal: *Unveiling the true band gap of fluorographene and its origins by teaming theory and experiment*. Applied Surface Science, 2022. DOI 10.1016/j.apsusc.2022.152839, IF 7.392 (JIMP)
- Giri Lopamudra, Rout Smruti Rekha, Varma Rajender S., Otyepka Michal, Jayaramulu Kolleboyina, Dandela Rambabu: *Recent advancements in metal-organic frameworks integrating quantum dots (QDs@MOF) and their potential applications*. Nanotechnology Reviews, 2022. DOI 10.1515/ntrev-2022-0118, IF 6.739 (JIMP)
- Panacek David, Zdrzil Lukas, Langer Michal, Sedajova Veronika, Bad'ura Zdenek, Zoppellaro Giorgio, Yang Qiuyue, Nguyen Emily P., Alvarez-Diduk Ruslan, Hruby Vitezslav, Kolarik Jan, Chalmpes Nikolaos, Bourlinos Athanasios B, Zbořil Radek, Merkoci Arben, Bakandritsos Aristeidis, Otyepka Michal: *Graphene Nano-beacons with High-Affinity Pockets for Combined, Selective, and Effective*

- Decontamination and Reagentless Detection of Heavy Metals*. Small, 2022. DOI 10.1002/smll.202201003, IF 15.153 (JIMP)
- Kadam Ravishankar G., Ye Tian-Nan, Zaoralová Dagmar, Medved Miroslav, Sharma Priti, Lu Yangfan, Zoppellaro Giorgio, Tomanec Ondřej, Otyepka Michal, Zbořil Radek, Hosono Hideo, Gawande Manoj B.: *Intermetallic Copper-Based Electride Catalyst with High Activity for C-H Oxidation and Cycloaddition of CO<sub>2</sub> into Epoxides*. Small, 2022. DOI 10.1002/smll.202201712, IF 15.153 (JIMP)
- Shi Yu, Wei Bo, Legut Dominik, Du Shiyu, Francisco Joseph S., Zhang Ruifeng: *Highly Stable Single-Atom Modified MXenes as Cathode-Active Bifunctional Catalysts in Li-CO<sub>2</sub> Battery*. Advanced Functional Materials, 2022. DOI 10.1002/adfm.202210218, IF 19.924 (JIMP)
- Obratsov Ievgen, Bakandritsos Aristeidis, Sedajova Veronika, Langer Rostislav, Jakubec Petr, Zoppellaro Giorgio, Pykal Martin, Presser Volker, Otyepka Michal, Zbořil Radek: *Graphene Acid for Lithium-Ion Batteries-Carboxylation Boosts Storage Capacity in Graphene*. Advanced Energy Materials, 2022. DOI 10.1002/aenm.202103010, IF 29.698 (JIMP)
- Lo Rabindranath, Manna Debashree, Hobza Pavel: *P-Doped graphene-C-60 nanocomposite: a donor-acceptor complex with a P-C dative bond*. Chemical Communications, 2022. DOI 10.1039/d1cc05737e, IF 6.065 (JIMP)
- Saini H., Otyepková E., Schneemann A., Zbořil Radek, Otyepka Michal; Fischer R.A., Jayaramulu K.: *Hierarchical porous metal-organic framework materials for efficient oil-water separation*. Journal of Materials Chemistry A. 2022. DOI 10.1039/d1ta10008d, IF 14.511 (JIMP)
- Chronopoulos Demetrios D., Stangel Christina, Scheibe Magdalena, Cepe Klara, Tagmatarchis Nikos, Otyepka Michal: *Electrocatalytic activity for proton reduction by a covalent non-metal graphene-fullerene hybrid*. Chemical Communications, 2022. DOI 10.1039/d2cc02272a, IF 6.065 (JIMP)
- Lin C., Feng X., Legut Dominik, Liu X., Seh Z.W., Zhang R., Zhang Q.: *Discovery of Efficient Visible-light Driven Oxygen Evolution Photocatalysts: Automated High-Throughput Computational Screening of MAZ<sub>4</sub>*. Advanced Functional Materials, 2022. DOI 10.1002/adfm.202207415, IF 19.924 (JIMP)
- Nieves Cordones Pablo, Arapan Sergiu, Zhang Shihao, Kadzielawa Andrzej Piotr, Zhang Ruifeng, Legut Dominik: *MAELAS 2.0: A new version of a computer program for the calculation of magneto-elastic properties*. Computer Physics Communications, 2022. DOI 10.1016/j.cpc.2021.108197, IF 4.717 (JIMP)
- Flauzino Jose M. R., Nguyen Emily P, Yang Qiuyue, Rosati Giulio, Panacek David, Brito-Madurro Ana G., Madurro Joao M., Bakandritsos Aristeidis, Otyepka Michal, Merkoci Arben: *Label-free and reagentless electrochemical genosensor based on graphene acid for meat adulteration detection*. Biosensors and Bioelectronics, 2022. DOI 10.1016/j.bios.2021.113628, IF 12.545 (JIMP)



- Chronopoulos Demetrios D., Saini Haneesh, Tantis Iosif, Zbořil Radek, Jayaramulu Kolleboyina, Otyepka Michal: *Carbon Nanotube Based Metal-Organic Framework Hybrids From Fundamentals Toward Applications*. Small, 2022. DOI 10.1002/sml.202104628, IF 15.153 (JIMP)
- Kiehbardrouinezhad Mohammadali, Merabet Adel, Rajabipour Ali, Čada Michal, Kiehbardrouinezhad Shahideh, Khanali Majid, Hosseinzadeh-Bandbafha Homa: *Optimization of wind/solar energy microgrid by division algorithm considering human health and environmental impacts for power-water cogeneration*. Energy Conversion and Management, 2022. DOI 10.1016/j.enconman.2021.115064, IF 11.533 (JIMP)
- Koleják Pierre, Lezier Geoffrey, Postava Kamil, Lampin Jean François, Tiercelin Nicolas, Vanwolleghem Mathias: *360° Polarization Control of Terahertz Spintronic Emitters Using Uniaxial FeCo/TbCo<sub>2</sub>/FeCo Trilayers*. ACS Photonics, 2022. DOI 10.1021/acsp Photonics.1c01782, IF 7.077 (JIMP)
- Hruby Vitezslav, Zaoralová Dagmar, Medved Miroslav, Bakandritsos Aristeidis, Zbořil Radek, Otyepka Michal: *Emerging graphene derivatives as active 2D coordination platforms for single-atom catalysts*. Nanoscale, 2022. DOI 10.1039/d2nr03453k, IF 8.307 (JIMP)
- Jayaramulu K., Mukherjee S., Morales D.M., Dubal D.P., Nanjundan A.K., Schneemann A., Masa J., Kment Štěpán, Schuhmann W., Otyepka Michal, Zbořil Radek, Fischer R.A.: *Graphene-Based Metal-Organic Framework Hybrids for Applications in Catalysis, Environmental, and Energy Technologies*; Chemical Reviews, 2022. DOI 10.1021/acs.chemrev.2c00270, IF 72.087 (JIMP)
- Lo Rabindranath, Manna Debashree, Lamanec Maximilian, Dracinsky Martin, Bour Petr, Wu Tao, Bastien Guillaume, Kaleta Jiri, Miriyala Vijay Madhav, Spirko Vladimir, Masinova Anna, Nachtigallová Dana; Hobza Pavel: *The stability of covalent dative bond significantly increases with increasing solvent polarity*. Nature Communications, 2022. DOI 10.1038/s41467-022-29806-3, IF 17.694 (JIMP)

#### Big Data Analysis Lab

- Nguyen Tan N., Tran Dinh-Hieu, Van Chien Trinh, Phan Van-Duc, Vozňák Miroslav, Tin Phu Tran, Chatzinotas Symeon, Ng Derrick Wing Kwan, Poor H. Vincent: *Security-Reliability Tradeoff Analysis for SWIPT- and AF-Based IoT Networks With Friendly Jammers*. IEEE Internet of Things Journal, 2022. DOI 10.1109/JIOT.2022.3182755, IF 10.238 (JIMP)
- Fazio Peppino, Mehić Miralem, Vozňák Miroslav: *An Innovative Dynamic Mobility Sampling Scheme Based on Multiresolution Wavelet Analysis in IoT Networks*. IEEE Internet of Things Journal, 2022. DOI 10.1109/JIOT.2021.3126550, IF 10.238 (JIMP)
- Thanh-Nam Tran, Thanh-Long Nguyen, Vozňák Miroslav: *Approaching K-Means for Multiantenna UAV Positioning in Combination With a Max-SIC-Min-Rate Framework to Enable Aerial IoT Networks*. IEEE Access, 2022. DOI 10.1109/ACCESS.2022.3218799, IF 3.476 (JIMP)

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Results of the last evaluation based on the MI module of the RIV 2017+ Methodology rated with grades 1–3

#### Advanced Data Analysis and Simulations Lab

- Tomčala J.: TSEntropies. 2019 (software)
- Böhm S., Beránek J.: RSDS. 2022 (software)

#### Advanced Data Analysis and Simulations Lab / Infrastructure Research Lab

- Křenek J., Svatoň V., Martinovič J., Konvička J., Jaroš M., Moravec V.: High-end Application Execution Middleware v2. 2022 (software)

# Advanced Data Analysis and Simulations Lab

The lab specialises in advanced data analysis, research and development in HPC co-design, data analysis and cloud technologies to enhance industry and society, programming models for HPDA, artificial intelligence, quantum computing, modelling, simulation, and application of dynamical systems.

Head of Lab  
Number of employees

Dr Jan Martinovič  
41.16 FTE

## Significant activities

- Launch of two Horizon Europe projects – [BioDT](#) coordinated by the Finnish CSC and [OpenWebSearch.EU](#) coordinated by German Universität Passau.
- The [hackathon](#) to develop the FIJI software for bioimage processing was held in Prague. The initiator of the event was Vladimír Ulman.
- The lab developed and upgraded specialised software packages for easier and faster protein research within the [PerMed Centre](#) project. The software, made available free of charge to researchers, opens up new possibilities for drug design.
- Collaboration with the Police of the Czech Republic in developing [models to predict criminality](#) and socio-pathogenic behaviour in the Czech Republic.
- Successful development of the [HyperQueue](#) tool, which facilitates the use of supercomputers with complex resources and provides a simple interface for scheduling computational tasks.
- Successful final review and transition to the sustainability phase of the Horizon 2020 [LEXIS](#) project. LEXIS was coordinated by this lab, and the LEXIS platform is used in other research projects.
- The LEXIS platform and the HyperQueue tool are used in the BioDT project and are an integral part of its implementation. These tools are gaining recognition on a European scale. The possibility of using the LEXIS platform is being evaluated, e.g., in the Digital Twin Ocean project.
- Acceptance of the Horizon Europe [EXA4MIND](#) project proposal coordinated by IT4Innovations.
- Collaboration in the submission and acceptance of the LUMI-Q project proposal.
- Successful completion of the [Bioimage Informatics](#) research programme, which was part of the IT4Innovations National Supercomputing Centre – the Path to Exascale project. The research programme was successfully presented and defended in front of expert evaluators and representatives of the grant provider.
- Release of the deterministic version of the IT4Innovations traffic simulator within the Horizon 2020 EVEREST project.
- A new [HEAppE middleware version](#) was released to support local HPC cluster simulation environments focused on local computing functions.
- Georg Zitzlsberger obtains two [NVIDIA Deep Learning Institute](#) certificates for AI – Applications of AI for Anomaly Detection and Applications of AI for Predictive Maintenance.

# Infrastructure Research Lab

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

Head of Lab  
Number of employees

Doc. Lubomír Říha  
15.54 FTE

## Significant activities

- Markéta Hrabánková, Ondřej Meca, Tomáš Brzobohatý (Parallel Algorithms Research Lab), Lubomír Říha, Milan Jaroš, and Petr Strakoš receive the [Best Research Poster Award](#) for their contribution entitled Toward Scalable Voxelization of Meshes with High Growth Rate at the SC22 Conference held in Dallas, Texas, USA.
- Acceptance of two [European Centres of Excellence](#) project proposals funded by the European Union and supported by the EuroHPC Joint Undertaking (MaX3 and SPACE), where IT4Innovations will be involved.
- Launch of the EuroHPC JU – project EUPEX, coordinated by the French Atos company (Bull SAS).
- Preparation and organisation of training courses – “Introduction to Performance and Energy Efficiency Analysis” and “Introduction to HPC” within the PRACE Training Centre, the “CUDA programming course” within the e-INFRA CZ project, EuroCC training course for a newly developed Medical-as-a-Service, and “Introduction to Parallel Programming”, a one-day course within the international Sctrain project.
- Being accepted for funding by the TREND programme of the Technology Agency of the Czech Republic, “[Combination of holographic and digital safety protection](#)” project submitted in cooperation with the Modelling for Nanotechnologies Lab.
- Development of [performance and power consumption monitoring of IT4Innovations supercomputers](#) (Karolina and Barbora), including correlation with PBS jobs.
- Definition of a [methodology for improving the energy efficiency](#) of IT4Innovations systems.
- Invited lectures at the Austrian-Slovenian HPC Meeting 2022 (ASHPC22) and HPCSE 2022.
- Kristian Kadlubiak successfully completed the Train the Trainer certified programme focused on parallel programming under the auspices of [Höchstleistungsrechenzentrum](#) Stuttgart (HLRS).

# Parallel Algorithms Research Lab

The laboratory is primarily focused on providing support for industry. The research team conducts applied research in developing scalable algorithms and HPC libraries, numerical modelling and simulations, and the deployment of artificial intelligence in engineering.

Head of Lab  
Number of employees

Dr Tomáš Karásek  
16.15 FTE

Significant activities

- In 2022, cooperation with Siemens s.r.o. and Orgrez a.s. continued on the projects “[Digital twin product at Siemens manufacturing plants](#)” and “[Research and development of application SW tool for effective evaluation of catalytic processes](#)”.
- The EuroCC project, under the auspices of which the [National Competence Centre in HPC \(NCC\)](#) was founded and operated, was completed. In the three years of its existence, the NCC prepared almost a dozen educational events and established a number of successful collaborations not only with industry. The EuroCC2 project was prepared and submitted to ensure the continuation of the NCC.
- Tomáš Brzobohatý and his colleagues from the Infrastructure Research Lab won the [Best Scientific Poster at the SC22 conference](#) in Dallas, USA, with their paper “[Toward Scalable Voxelization of Meshes with High Growth Rate](#)”.
- Active participation in organising the High Performance Computing in Science and Engineering ([HPCSE 2022](#)) conference.
- In March 2022, the PRACE Summer of HPC 2021 Internship Awards were announced during the EuroHPC Summit Week conference. The [PRACE Summer of HPC 2021 HPC Ambassador Award](#) went to students Jenay Patel from the University of Nottingham, UK, and Carola Ciaramelletti from the Università degli studi dell'Aquila, Italy, who studied molecular dynamics on quantum computers under the guidance of Martin Beseda and Stanislav Paláček as their mentors.
- Zaoral F.: Development of a software tool for automation of pre-processing in analysis using the Finite Element/Methods; 017/30-11-2022\_SW; 2022.
- Hrabánková M., Meca O., Jaroš M., Brzobohatý T., Říha L., Strakoš P.: Parallel voxelization of unstructured meshes for volume rendering; 029/14-12-2022\_SW; 2022.
- Meca O., Brzobohatý T., Říha L.: Parallel loading of unstructured meshes in Neper format; 026/14-12-2022\_SW; 2022.
- In cooperation with the Middle East Technical University, a course on “[High Performance CFD using OpenFOAM](#)” was prepared and organised, attended by 90 people.

# Modelling for Nanotechnologies Lab

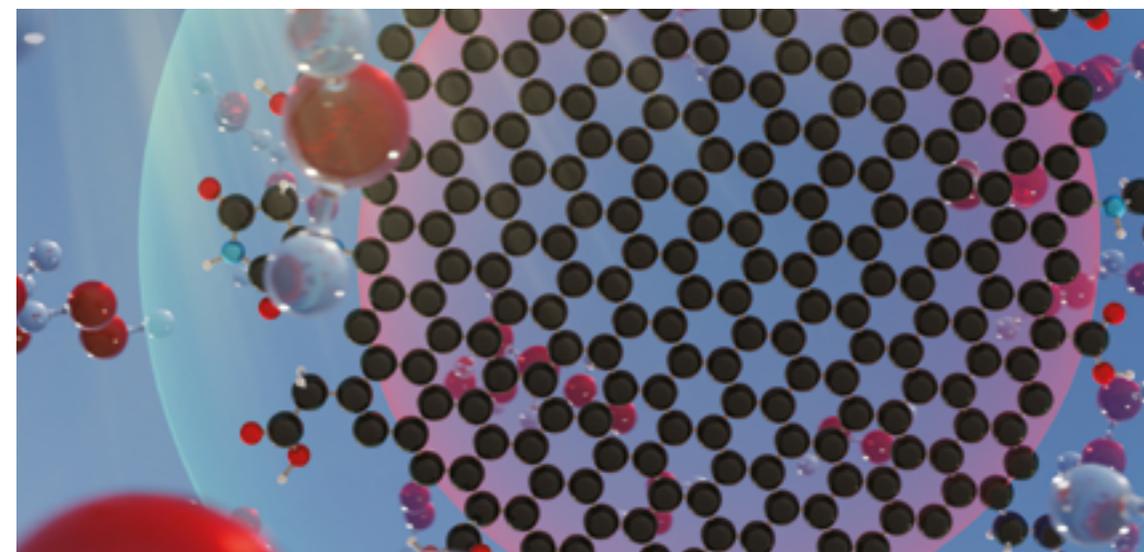
The Lab focuses on design, computer modelling, and preparation and experimental characterisation in the field of advanced nanomaterials and nanotechnology. It is also dedicated to developing special surfaces for nano-optics and has state-of-the-art experimental equipment for studying nanosystems.

Head of Lab  
Number of employees

Prof. Michal Otyepka  
19.05 FTE

Significant activities

- Scientists from several Czech research institutes, including IT4Innovations, developed a [new anode for lithium-ion batteries](#) based on graphic acid – a densely carboxylated graphene derivative.
- Lukáš Halagačka completed an internship focused on the study of silicon nanowire structures for the preparation of solar cells at the [prestigious École Polytechnique in Palaiseau](#).
- A new, cheap, efficient, and recyclable material capable of [detecting and eradicating heavy metals](#) in water was developed by IT4Innovations researchers in collaboration with scientists from several research centres.
- Prof. [Pavel Hobza](#), a member of the Modelling for Nanotechnologies Lab, won the [Neuron Endowment Fund Prize](#) in chemistry.



↔ Author of the picture: Martin Pykal



# Big Data Analysis Lab

The laboratory is focused on network security, the Internet of Things, big data analysis, speech processing, and artificial intelligence applications in complex systems. It also aims to develop efficient knowledge acquisition and processing methods.

Head of Lab  
Number of employees

Prof. Miroslav Vozňák  
3.54 FTE

Significant activities

- The continuation of the Horizon 2020 [OpenQKD](#) (Open European Quantum Key Distribution Testbed) project, which aims to create a testbed for a highly secure network using quantum mechanical principles for key distribution while strengthening the security of critical applications in telecommunications, healthcare, energy, and many other strategic sectors.
- Work on the [Artificial Intelligence and Reasoning](#) project supported by the MEYS of the Czech Republic, which deals with artificial intelligence methods in automatic reasoning, formal verification of theories and systems, planning and scheduling and their industrial applications, complex systems, and computational linguistics.



↔ [Karolina](#)

The Karolina supercomputer was the 69<sup>th</sup> most powerful supercomputer at its launch, according to the TOP500 ranking.

# 6

## Educational and Training Activities

IT4Innovations has long been involved in a wide range of educational and training activities. Each year it offers around 20 courses, workshops, and conferences focused on HPC, HPDA, QC, and AI. The courses are not only led by IT4Innovations experts, but also by lecturers from leading international institutions.

### Educational activities

IT4Innovations and the Faculty of Electrical Engineering and Computer Science of VSB-TUO prepared and successfully accredited the **Informatics and Computational Science** PhD study programme, which is focused, among others, on using HPC, HPDA, and AI in science and industry. In 2022, 22 students were enrolled in the ongoing PhD programme in Computational Sciences, with two of them successfully completing their studies. The programme is part of the **MathInHPC Doctoral School** ([www.mathinhpc.cz](http://www.mathinhpc.cz)), which brings together leading Czech institutes

focused on research in mathematical methods in HPC and their applications. Its students thus also have an opportunity to select from the joint portfolio of study courses as well as the dissertation topics provided by the participating institutions and under their joint supervision, respectively. The partners of the Doctoral School include, for example, the Faculty of Mathematics and Physics of Charles University and the Institute of Mathematics of the Czech Academy of Sciences.

IT4Innovations is intensely engaged in teaching within the Computational and Applied Mathematics MSc study programme, guaranteed by the Department of Applied Mathematics at the Faculty of Electrical Engineering and Computer Science of VSB-TUO. In 2022, our colleagues from the Advanced Data Analysis and Simulations Lab prepared the Introduction to Quantum Computing course, which will be studied by the first students of the Faculty of Electrical Engineering and Computer Science at VSB-TUO in 2023.

In addition, IT4Innovations is a member of an international consortium that is implementing the very first pan-European Master's study programme focused purely on High-Performance Computing – **EUMaster4HPC**. The consortium, led by the University of Luxembourg, includes universities, research and supercomputing centres, industrial partners, and other cooperating institutions. Starting from the 2022 winter semester, the MSc study programmes are provided by eight European universities. Participation of the Czech Republic in the pan-European EuroHPC Joint Undertaking enables Czech students to also enroll for this study programme. Graduates will find careers in fast-growing fields such as HPC, HPDA, and artificial intelligence. This project is part of a more comprehensive EuroHPC JU strategy facilitating the development of key capabilities as well as education and training in the field of HPC to meet the needs of European science and industry.

### Training activities

IT4Innovations supports the scientific community and its users by organising high-quality courses, tutorials, workshops, and other training events. The primary objective of these activities is to broadly enhance users' competencies in terms of efficient use of the unique IT4Innovations supercomputing infrastructure. In a broader sense, IT4Innovations aims to increase the awareness and knowledge of HPC nationwide among interested members of academia and industry. The training activities also have a Europe-wide reach as they are open to the European community within the framework of international projects in which IT4Innovations has participated and is participating, such as PRACE, EuroCC, IO-SEA, and others. Thematically, the courses offered by IT4Innovations focus on computer systems and architecture, programming techniques and tools, libraries and applications in HPC, HPDA, AI, and quantum computing.

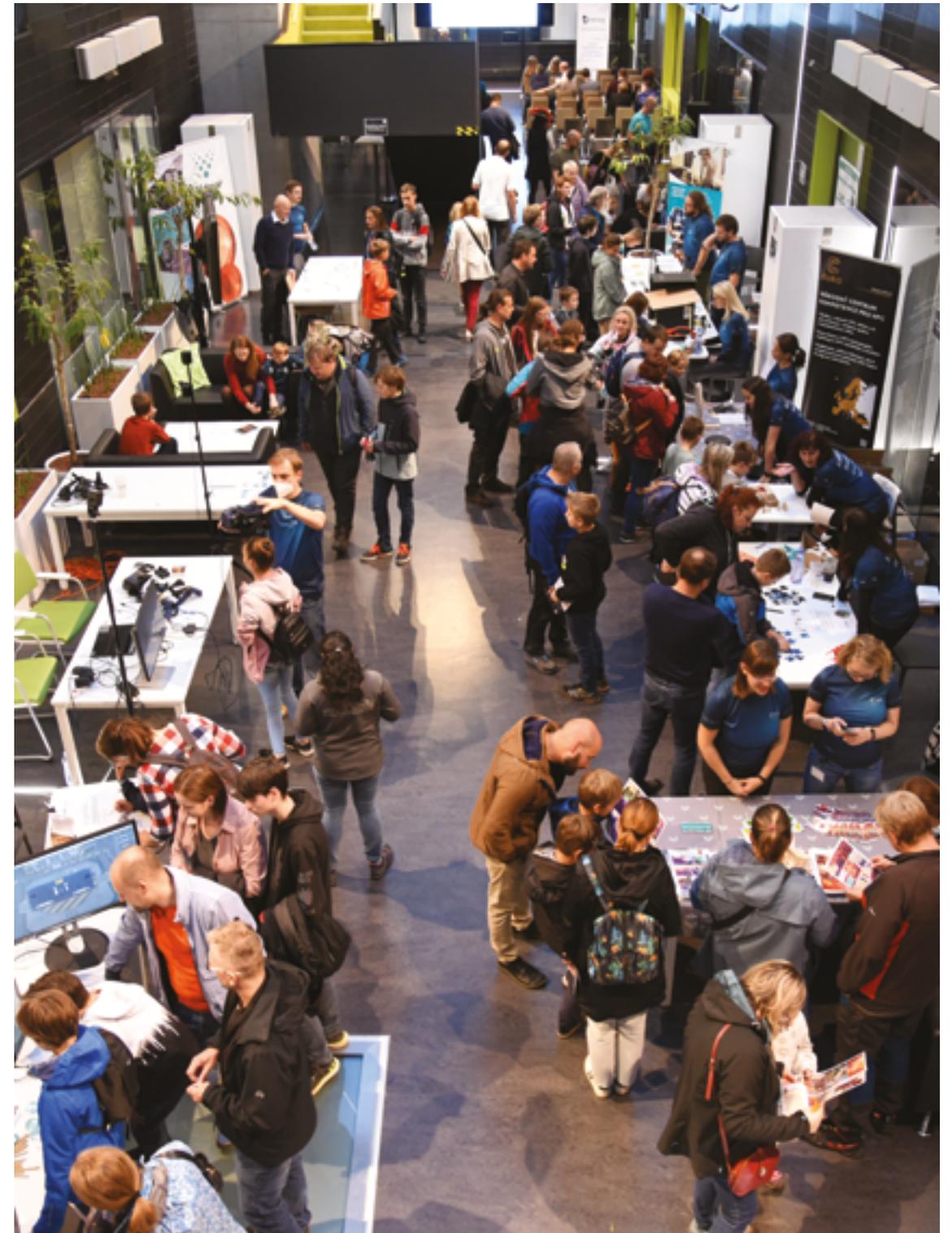
In 2022, IT4Innovations held 17 educational events and workshops attended by 540 participants, whether in person or online. Compared to previous years, this is a more than two-fold increase. Seven of them were held under the auspices of the PRACE project, as IT4Innovations has been a PRACE Training Centre (PTC) since 2017, six under the EuroCC project, two under the IO-SEA project, and one under the Sctrain project.

- [Fundamentals of Deep Learning](#) (PTC course), 4<sup>th</sup> January, online, 29 participants
- [Building Transformer-Based Natural Language Processing Applications](#) (PTC course), 5<sup>th</sup> January, online, 25 participants
- [SCtrain – Introduction to Parallel Programming](#), 31<sup>st</sup> January–4<sup>th</sup> February, online, 39 participants
- [Introduction to Machine and Deep Learning](#) (PTC course), 15<sup>th</sup> March, online, 28 participants
- [Introduction to Performance and Energy Efficiency Analysis](#) (PTC course), 5<sup>th</sup> April, online, 19 participants
- [High Performance CFD using OpenFOAM](#) (EuroCC course), 28<sup>th</sup> April, online, 90 participants
- [Data Science with R and Python](#) (PTC course), 12<sup>th</sup> May, online, 30 participants
- [Introduction to Atos QLM and how to use it to run your first quantum circuit](#) (EuroCC course), 25<sup>th</sup> May, online, 15 participants
- [Fundamentals of Deep Learning using MultiGPUs](#) (EuroCC course), 8<sup>th</sup> June, online, 22 participants
- [Introduction to HPC](#) (PTC course), 14<sup>th</sup> June, online, 18 participants
- [GPU programming: CUDA](#) (e-INFRA CZ), 7<sup>th</sup> October, onsite, 7 participants
- [IO-SEA: Software for Exascale Architectures Driven by Hierarchical Storage Management Approach](#), 13<sup>th</sup> October, online, 37 participants
- [Quantum computing for secondary schools' workshop](#) (EuroCC course), 21<sup>st</sup> October, onsite, 33 participants
- [Quantum Computing Workshop: Hybrid Systems](#) (EuroCC course), 25<sup>th</sup> November, online, 80 participants
- [Introduction to Machine and Deep Learning](#) (EuroCC course), 29<sup>th</sup> November, hybrid form, 21 participants
- [IO-SEA: Cortx Motr Object Storage](#), 6<sup>th</sup> December, hybrid form, 28 participants
- [Parallel Programming with OpenMP](#) (PTC course), 7<sup>th</sup>–8<sup>th</sup> December, online, 19 participants

## PRACE Summer of HPC

As part of the PRACE project and its sixth implementation phase, students had the opportunity to participate in summer internships in European supercomputing centres for the tenth time in 2022. In this latest edition in summer 2022, 29 students working on 22 projects took the opportunity to experience a summer internship in a supercomputing centre. IT4Innovations hosted four of them.

Monika Das from the French University of Bourgogne-Franche-Comté and Leo Lassalle from the French Polytech Sorbonne worked on the Fundamentals of Quantum Algorithms and their Implementation project under the supervision of Jiří Tomčala. The second team of students was led by Dominik Legut. Under his supervision, Luigi Camerano Spelta Rapini and Mattia Iannetti from the Italian University of L'Aquila worked on his Heat Transport in Novel Nuclear Fuels project.



↔ [Researcher's Night](#)

The evening event, during which hundreds of scientific workplaces open their doors to the public, took place on Friday 30 September, and attracted 900 visitors to IT4Innovations.

# 7

## List of Projects

### National Projects

#### Supercomputing Services Projects

Projects supported by the Ministry of Education, Youth and Sports of the Czech Republic  
Large Infrastructures for Research, Experimental Development and Innovation project

#### e-Infrastructure CZ (2020–2022)

→ Project ID: LM2018140  
→ 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 and international levels. It also provides an extensive and comprehensive portfolio of ICT services for conducting modern research, development and innovation.

The main components of e-INFRA CZ include:

- high-performance national communication infrastructure,
- national grid and cloud infrastructure,
- most powerful and state-of-the-art supercomputing systems in the Czech Republic,
- high-capacity data storage facilities.

Other tools and services, such as access control to ICT resources, tools to support remote cooperation, and tools to ensure secure communication and data protection, are also an essential part and an added value of this infrastructure, contributing to its efficient and diverse use. Jinou spoluprací nebo nástroje pro zajištění bezpečné komunikace a ochrany dat, které společně přispívají k jejímu efektivnímu a současně různorodému využití.

#### Operational Programme Research, Development and Education Projects

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

- Project ID: EF16\_013/0001791
- Principal Investigator: Dr Branislav Jansík

→ This project aimed to upgrade and modernise the IT4Innovations research infrastructure to maintain the existing technological level of HPC in the Czech Republic compared to developed, mainly 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, the Karolina supercomputer was procured, exceeding the capacity of Salomon, the previously most powerful system of IT4Innovations.

The project also supported excellent research of the broad academic community in the Czech Republic and the expansion of existing research activities at IT4Innovations in the areas of the modelling of photonic and spin-photonic structures, design of new progressive materials based on electronic structure calculations and analysis of biological images using HPC. In-house research is an essential source of HPC expertise for IT4Innovations, reflected in the infrastructure's services to its users.

#### e-INFRA CZ: Modernisation (2020–2023)

- Project ID: CZ.02.1.01/0.0/0.0/18\_072/0015659
- Principal Investigator: Dr Branislav Jansík

→ The project aims to modernise and provide the necessary capacities within specific 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, simultaneously, to the state-of-the-art level of the field. The project focuses primarily on the complete upgrade of all layers of the standard 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 equivalent units in the European (GÉANT, EGI, EOSC, EuroHPC, ETP4HPC, EUDAT, PRACE, ...) and global (GLIF) R&D area and of course with related infrastructures and entities at the national level.

## Research and Development Projects

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

#### 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 was, among others, to extend IT4Innovations in-house research in the three following fields: 1) Modelling of photonic and spin-photonic structures, design of novel progressive materials based on electronic structure calculations, and bioimage analysis using HPC. In-house research is an essential source of HPC expertise for IT4Innovations, reflected in the infrastructure's services to its users. 2) Use of approximations involving many-body effects (MB) in electrons. Further, it was the inclusion of temperature effects in computational methods, particularly anharmonic lattice vibration effects, and thus the possibility to study materials in near-realistic conditions. Finally, it was the possibility and access to study 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 they exist in natural materials and often limit their use. 3) Creating a globally unique platform for analysing biological and biomedical image data using the open-source Fiji platform's high-performance computing (HPC) infrastructure.

#### Artificial Intelligence and Reasoning (2017-2023)

→ Project ID: CZ.02.1.01/0. 0/0.0/15\_003/0000466

→ Principal Investigator: Prof. Václav Snášel

→ The project yielded significant measures for developing informatics, robotics, and cybernetics research at the Czech Technical University in Prague. The project established a new AI and Reasoning research group within a given part of the Czech Institute of Informatics, Robotics, and Cybernetics (CIIRC), which focused on solving advanced interdisciplinary problems of high technical as well as social priority. The project was also supported by national partners (VSB-TUO and the University of West Bohemia in Pilsen). The motivation for their participation stems from the emphasis not only on the concentration and integration of resources and sharing of knowledge and infrastructure but also on establishing a “unified space for opportunities” for young talents in the Czech Republic.

#### Modelling of Collision Processes in Low-Temperature Plasma (2021-2022)

→ Project ID: DGS/TEAM/2020-020

→ Principal Investigator: Martin Beseda

→ The project represented a part of a broader research outlook, in collaboration with Université Toulouse III – Paul Sabatier (UPS), focused on investigating low-temperature rare-gas-based plasma for (most importantly) biomedical applications. It covered two double-degree dissertation theses (those of Beseda and Fresnelle) and two other theses (of Horáčková and Paláček). The project focused on modelling plasma interactions with air as the first step towards understanding the interactions between plasma active species with biomedical substrates. This project followed the previous research efforts (one co-supervised thesis, one double-degree thesis, and approximately eleven published papers).



↔ A visit from the European Union

In July, ambassadors from the Committee of the Permanent Representatives of the Governments of the Member States to the European Union visited IT4Innovations.

**Development of a tool for scientific data processing and visualisation in VR with multi-user support (2021-2023)**

- Project ID: DGS/TEAM/2020-008
- Principal Investigator: Markéta Hrabánková
- There is an ever-increasing need to visualise data from large computations on HPC systems. Monitoring such systems during their runtime and visualising this information properly is important. To explore the data more intuitively, it is desirable to use 3D visualisations. For this purpose, we aim to create open-source tools that will allow data to be processed and visualised in high quality and support its presentation in virtual reality (VR). The developed tools will be specifically focused on medical data visualisation, HPC cluster runtime monitoring, and the visualisation of simulation results from parallel open-source simulation tools. High-quality visualisations in VR are the primary goal of the project. Another goal is to strengthen cooperation among researchers with different specialisations.

The project will also enable and visualise resource consumption monitoring of IT4Innovations and their visualisation. This feature, which will be greatly appreciated by both administrators and users of these systems, will allow for follow-up research based on the data collected, such as research into energy-aware job scheduling.

**Novel sources of THz radiation based on spintronic effects (2021-2023)**

- Project ID: DGS/TEAM/2020-027
- Principal Investigator: Pierre Koleják
- The terahertz (THz) spectral range holds immense potential for medical, security, and telecommunications applications. Therefore, it is desirable to develop new sources of terahertz waves with fast response, intense signal, controlled polarisation properties, and easy implementation. In this project, terahertz sources using spintronic phenomena such as terahertz spintronic emitters based on the spin-Hall effect and spin-laser-based THz sources will be designed, developed, and characterised. Photonic and plasmonic structures will be employed to enhance the performance of these devices, including Bragg grating and plasmonic materials for spintronic emitters and anisotropic 2D grating for spin lasers. Nonconventional characterisation methods will be used to describe spin mobility and broadband optical properties, including terahertz plasma-based time-domain spectroscopy and pump-probe terahertz measurements. Numerical simulations of ultrafast dynamics and spin transport will allow a deeper understanding of spin-based generation processes. The project is highly interdisciplinary, including approaches and methods from optics, magnetism, engineering, advanced nanotechnology, high-performance computing modelling, and applied quantum theory.

**Development of Computational Algorithms for Solution of Non-linear Structural Dynamical Problems with Utilisation of ESPRESO Numerical Library (2021-2023)**

- Project ID: DGS/TEAM/2020-033
- Principal Investigator: Michal Molčan
- The proposed project aims to develop computational procedures to solve non-linear structural dynamical problems. Moreover, the procedures will be applied to computational models of rotating machinery, discretised by three-dimensional finite elements, to analyse their vibrations. Within the scope of this project, investigators will develop procedures for (i) steady-state response determination utilising the Harmonic Balance Method (HBM), (ii) determination of the amplitude-frequency response curve by the continuation technique, (iii) the stability

and essential bifurcation analysis of the steady-state response, (iv) the identification of an optimal strategy for the amplitude-frequency response curve determination by the application of Total Finite Element Tearing and Interconnecting (T-FETI) on a linearised model, including the application of suitable preconditioners and coarse space projectors, and, (v) the determination of the transient response of the model, based on corotational finite element formulation utilising time-integration. The procedures will be created and studied on the test cases in the MATLAB software and subsequently implemented in ESPRESO (ExaScale Parallel FETI Solver) developed as an open-source code project at IT4Innovations and tested on real industrial cases.

**Researcher Mobility Support within international cooperation in R&D&I**

**Multiscale design of novel Rare Earth free permanent magnets (2020-2022)**

- Project ID: 8X20050
- Principal Investigator: Dr Dominik Legut
- The research was a complementary joint work of the following institutions – VSB-TUO, Prešov University, and the Donau-University Krems. The project consisted in finding novel RE-free permanent magnets using 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 a uniaxial lattice, were further tested to see if they also show high magnetocrystalline anisotropy, exchange integrals ( $J$ 's), and temperature ( $T_C$ ) of transition from magnetic to paramagnetic state. First, MAE and  $J$ 's were obtained from the quantum mechanical calculations using HPC infrastructure, followed by  $T_C$  obtained from the atomic spin dynamics calculations. The structural parameters of the most stable candidates were transferred to the Slovak partners to synthesise samples and to measure the number of magnetic quantities like magnetisation, magnetic susceptibility, etc. At the same time, the Austrian partner performed micromagnetic simulations to determine the magnetic behaviour of given materials in terms of their texture, shape, and thickness under various thermal conditions.

**International cooperation in R&D&I**

**Influence of thermo-electrical effects on spin-orbit torques in 2D van der Waals materials (2022-2025)**

- Project ID: LUASK22099
- Principal Investigator: Dr Dominik Legut
- Two-dimensional materials provide a novel building platform for nanotechnology and functional nanodevices. The functional nanodevices, i.e., nano-sized devices, are expected to enter 21st-century modern society. One of them is a non-volatile magnetic memory element controlled by electrical current only involving anomalous effects (e.g., the anomalous Hall effect) due to spin-orbit coupling interaction in materials or on their interfaces. The project builds on the assumption that such an element contains a magnetic part for storing the information and a non-magnetic part with strong spin-orbit coupling, which allows the spin-orbit torque to control the magnetisation dynamics, i.e., reading and writing information. A key question addressed within this project is how the Joule heat produced due to the flow of current in such a nanodevice affects the spin-orbit torque. The project aims at exploring and explaining the proximity and temperature effects on spin-orbit torque in devices made of 2D materials forming van der Waals heterostructures. The experience and computational procedures of both partners (VSB-TUO and

Pavol Jozef Šafárik University in Košice) will be applied to determine the thermoelectric phenomena and the influence of interfaces for experimentally relevant 2D spin-orbit torque systems.

#### Projects supported by the Moravian-Silesian Region

##### Individual projects

- Project ID: O8183 2019 RRC (S516/20-96100-01RN)
- Principal Investigator: Martin Duda

→ Financial support from the Moravian-Silesian Region was dedicated to the provision of discounted services related to the use of the IT4Innovations computational resources. This support was intended for small and medium-sized enterprises with a registered office or branch in the Moravian-Silesian Region and was provided under a de minimis regime. This support enabled progressive small and medium-sized enterprises, including start-ups, to use supercomputing technologies and expertise to develop their business activities.

#### Projects supported by the Grant Agency of the Czech Republic

##### International grant projects evaluated by the LEAD Agency

- Project ID: 22-35410K
- Principal Investigator: Dr Dominik Legut

→ Permanent magnets are a key technology for modern society with applications in air conditioning, mobility, and power generation. In state-of-the-art permanent magnets, the atomic-scale defects, like in the grain boundary phase, have the most significant effects on the macroscopic properties (e.g., coercivity). In this project, a quantitative theory of coercivity, in terms of the local atomic structure, the spatial variation of the intrinsic magnetic properties, and the physical microstructure of the magnet will be studied. To achieve this goal, a unique scheme of simulation procedures will be developed between quantum mechanical calculations, atomic spin dynamics, and micromagnetic continuum simulations. Magnetic properties will, therefore, be newly taken into account on the atomic scale, i.e., with the inclusion of atomic interface defects and grain boundaries. This will avoid the use of former assumptions in the use of magnetic properties from solid phases. This will allow a multi-scale model to be built to determine the magnetic properties of real materials.

##### Standard grant projects

- Project ID: 20-18392S
- Principal Investigator: Dr Andrzej Kądziaława

→ The project dealt with the physical principles that will increase the phase stability region between the immiscibility and melting temperatures using an example of desired alloys with a self-passivation role for fusion reactor vessels. A phase diagram of the W-Cr system was constructed using first-principles methods, and the

physical properties (speed of sound, melting temperature, immiscibility region) were determined. Both the phase diagram and these quantities were verified experimentally. Enriching the alloy with transition metals from the sixth period changed the phases' melting and miscibility. The project's main idea is to determine the change in these temperatures based on the change in the acoustic branches of the added element's phonon spectrum (elasticity). Using XRD analysis and RUS measurements of the experimental samples, data was obtained to provide feedback for theoretical modelling to develop an alloy able to withstand a "Loss of Coolant Accident". Furthermore, a physical model based on the Hubbard Hamiltonian was derived to determine the influence of quantities such as entropy on the behaviour of the immiscibility region.

#### Unconventional superconductors under extreme conditions (2022-2024)

- Project ID: 22-22322S
- Principal Investigator: Dr Dominik Legut

→ The recently discovered superconductivity in the nearly magnetic compound UTe<sub>2</sub> boosted interest in unconventional superconductors. The results published so far indicate multiple superconducting phases and magnetic ordering induced by applying an external magnetic field and/or hydrostatic pressure. The revealed analogies of the behaviour of UTe<sub>2</sub> with the properties of ferromagnetic superconductors URhGe, UCoGe and UGe<sub>2</sub> may help develop a unified theory of unconventional superconductivity. The project will bring together experimentalists (Charles University) and theorists (VSB-TUO) to collaborate intensively in a comprehensive investigation of a complex phase diagram of UTe<sub>2</sub> and related compounds employing a yet unseen combination of experimental measurements and state-of-the-art theoretical ab initio calculations of thermal expansion, magnetostriction, heat capacity, magnetisation, elastic constants, and electrical transport of unconventional superconductors under multi extreme conditions.

#### Projects supported by the Technology Agency of the Czech Republic

##### National Competence Centres Programme

- Project ID: TN01000013
- Principal Investigator: Dr Jan Martinovič

→ The PerMed Centre was focused on applied research in the diagnostics and therapy of rare and genetically determined diseases. The aim was to develop personalised diagnostic methods and drugs that would help specific groups of patients. The highly interdisciplinary approach combined medicine, chemistry, biology, genetics, and bioinformatics. All research activities included molecular target validation, biological chemistry, preclinical development, biomarker identification, and DNA analyses. The results of the PerMed Center were commercialised both by licensing as well as the establishment of spin-offs.

#### Personalised Medicine - Diagnostics and Therapy (2019-2022)

#### Digital Innovation Hub - pilot verification (2020-2022)

#### Magnetism at interfaces: from quantum to reality (2022-2025)

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

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

TREND Programme

- Project ID: FW2020151
- Principal Investigator: Dr Kateřina Slaninová
- In compliance with the TREND programme, the main objective of the project was to increase the international competitiveness of the applicant Bonmedix Holding a.s., especially by penetrating markets in the EU and the USA with a newly developed service that will subsequently be certified as a medical device.

The main objective was 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 the diagnosis of diabetic retinopathy. The expert system used 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 was then clinically validated on real data.

**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 in simulated conditions (2020–2022)**

- Project ID: FW01010274
- Principal Investigator: Dr Petr Strakoš
- The project's main objective was 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 the final identification of obstacles and their interpretation for the locomotive driver. As a key support for developing and optimising the detection system, the project included developing a software simulator for virtualising railway conditions and implementing test rides in a laboratory environment.

ÉTA Programme

**Creating a model for evaluating the impact of changes in the parameters of the tax-benefit system on the socio-economic situation of families with children in the Czech Republic (2021–2023)**

- Project ID: TL05000184
- Principal Investigator: Prof. Marek Lampart
- The project aims to create a comprehensive research report and software for the needs of the Ministry of Labour and Social Affairs based on an in-depth and comprehensive analysis of the position of Czech households according to the type of household, the number of children, and the absolute and relative income in the context of the tax-benefit system. The outputs of the in-depth analysis will serve as essential material for creating a model of the tax-benefit system implemented in software, of which the primary purpose will be to monitor and empirically evaluate the impact of legislative changes in current Czech family policy in the tax-benefit system on the socio-economic status of particular households and numbers of children.

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

**Projects supported by the Ministry of Trade of the Czech Republic**  
Projects of the Operational Programme Enterprise and Innovation for Competitiveness

- Project ID: CZ.01.1.02/0.0/0.0/17\_176/0015651
- Principal Investigator: Dr Tomáš Brzobohatý
- The project aimed to research and develop the digital twin product at Siemens, s.r.o. The project was divided into two parts; the first part, i.e., the research and development of the digital twin product, an asynchronous electric motor, was conducted at the Siemens branch s.r.o. Elektromotory Frenštát.

**SmartFleet – AI based software for a full utilisation of electric cars in companies and maximisation of their share in the car fleet (2021–2023)**

- Project ID: CZ.01.1.02/0.0/0.0/20\_321/0024896
- Principal Investigator: Dr Kateřina Slaninová
- The project goal is to create a SmartFleet platform, which should enable optimisation of company car fleets in terms of their composition and utilisation to maximise the share of cars that use alternative fuels (especially electric cars). The solution will be developed as interdisciplinary and open, which allows flexibility in terms of new inputs (e.g., location of hydrogen stations in the future) and enables iteration when considering modification of the car fleet and solving complete car fleet lifecycles.

**Holograms with active safety elements (2021–2023)**

- Project ID: CZ.01.1.02/0.0/0.0/20\_321/0024953
- Principal Investigator: Dr Kamil Postava
- The aim of the joint industrial research project of Optaglio a.s. and VSB-TUO is to develop new products in the field of security holography that will be competitive on global markets. These are entirely new types of anti-counterfeiting features. In the framework of the presented project, we will focus on two original approaches to security holography, combining a high technical production level and advanced nanostructure design methods.

**Research and development of application SW tool for efficient evaluation of catalytic processes (2021–2023)**

- Project ID: CZ.01.1.02/0.0/0.0/21\_374/0026707
- Principal Investigator: Dr Tomáš Brzobohatý
- The project aims to create SW for the effective evaluation of catalytic processes and for comprehensive support in designing SCR technologies for industrial applications. The research and development activities solve the overall DeNOx process by reducing nitrogen oxides from the exhaust gases when reacting with gaseous NH3. The SW will be based on machine learning algorithms and flow calculations (CFD). The SW has a direct commercial application in nitrogen emission reduction solutions in power plants in both the Czech Republic and abroad.



↔ LUMI

In addition to the supercomputers operated by IT4Innovations, the Czech research community may also use the computational resources of the LUMI supercomputer, installed in Kajaani, Finland, since the end of 2021. Thanks to IT4Innovations' membership in the LUMI consortium, Czech scientists also have access to one of the world's most powerful and advanced supercomputers; the peak theoretical performance reached 428 PFlop/s in 2022.

**Development, security, and scalability of cloud services in the area of digital transformation (2021-2023)**

- Project ID: CZ.01.1.02/0.0/0.0/ 20\_321/0024591
- Principal Investigator: Dr Kateřina Slaninová

→ The project aims to conduct research and development activities in the area of cloud and printing solutions. The project will be implemented in effective collaboration of Y Soft: Print Management Solutions, a.s., with VSB-TUO and the Czech Technical University in Prague.

**Educational Projects**

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

Projects of the Operational Programme Research, Development and Education

- Project ID: CZ.02.2.69/0.0/0.0/16\_018/0002713
- Principal Investigator: Prof. René Kalus

→ The main objective of the project was the establishment of a Doctoral School for Education in Mathematical Methods and Tools in HPC, integrating doctoral studies at Charles University (Faculty of Mathematics and Physics), the Czech Academy of Sciences (Institute of Mathematics), and VSB-TUO and building on their broader research cooperation. Part of the project was the modernisation and internationalisation of one of the doctoral programmes of the Doctoral School (Computational Sciences, VSB-TUO) and the creation of a new double-degree programme in collaboration with Université Toulouse III Paul Sabatier in France. → [www.mathinhpc.cz](http://www.mathinhpc.cz)

**VSB-TUO projects with IT4Innovations participation**

**Projects of talented VSB-TUO PhD students (2019-2022)**

- Project ID: 07685/2019/RRC
- IT4I Coordinator: Prof. Tomáš Kozubek
- Grant Provider: MSR

→ The project aimed to support talented PhD students at VSB-TUO. The support of students was in the form of the payment of an additional contribution to the regular doctoral scholarship for students. VSB-TUO, in cooperation with the Moravian-Silesian Region, contributed to better conditions for students in their scientific activities, especially in relation to the use of the results of their scientific work in the application area.

**Technology for the Future 2.0 (2019-2022)**

- Project ID: CZ.02.2.69/0.0/0.0/18\_058/0010212
- IT4I Coordinator: Prof. Tomáš Kozubek
- Grant Provider: MEYS CR

→ The project enhanced educational activities' quality and profile and increased their relevance for the labour market. It implemented new forms of educational methods, established new study programmes, and boosted the internationalisation of the university and ties between the university and its graduates. It implemented methods for increasing the participation of students with special needs and improving the strategy for motivating secondary school students to enrol for tertiary education studies. It enhanced not only the capacities of the management

personnel of higher education institutions (HEI) but also the quality of the HEI strategy management. The project's main objective was 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's educational activities reflect the needs and unique features of the labour market in the MSR and of all target groups.

#### **Science without Borders 2.0 (2020–2023)**

- Project ID: CZ.02.2.69/0.0/0.0/18\_053/0016985
- IT4I Coordinator: Prof. Tomáš Kozubek
- Grant Provider: MEYS CR

→ The project will facilitate the mobility of 26 researchers of diverse nationalities to and from the Czech Republic. It will thus address the need for more international cooperation in research and the professional growth of human resources in research. Researchers will develop in their fields of study, 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.

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

- Project ID: VI20192022169
  - Principal Investigator: Petr Berglowiec (Faculty of Safety Engineering, VSB-TUO)
  - Grant Provider: MI CR
- This project focused on deploying artificial intelligence technologies for the automated reception and processing of emergency calls using a voice chatbot in speech analytics, semantic analysis, dialogue management, and voice synthesis are expected, including the integration of geographical data. The output was a functional demonstrator working with real telephone calls under the condition of immediate deployment in an Integrated Rescue System (IRS) and recommendations for system integration and its further development towards IRS automation.

#### **National Centre for Energy (2019–2022)**

- Project ID: TN01000007
  - Principal Investigator: Prof. Stanislav Mišák (ENET Centre, VSB-TUO)
  - Grant Provider: TA CR
- The National Centre for Energy (NCE) aimed to stimulate long-term cooperation among the leading research organisations and major application entities in the power industry. Consequently, unique infrastructures and know-how of expert teams of the existing research centres were shared by implementing joint applied research projects. The research agenda of the NCE was in line with the National RIS3 Strategy and focused on new technologies leading to the increased efficiency, safety, and reliability of existing energy units, the efficient deployment and operation of decentralised sources of energy, the use of alternative fuels to secure mineral resource independence and the energy self-sufficiency of the Czech Republic and the powering of grids safely and securely.

#### **Energy system for grids (2019–2023)**

- Project ID: TK02030039
- Principal Investigator: Prof. Stanislav Mišák (ENET Centre, VSB-TUO)
- Grant Provider: TA CR

→ The project aims to develop 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 sources 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 updated State Energy Conception.

#### **CEET – Center of Energy and Environmental Technologies (2020–2022)**

- Project ID: TK03020027
- Principal Investigator: Prof. Stanislav Mišák, (ENET Centre, VSB-TUO)
- Grant Provider: TA CR

→ The main objective of the project was the development of a modular, mobile, robust, and scalable technology solution for the efficient conversion of alternative fuels, waste, and by-products as alternative raw materials into usable chemicals and useful forms of energy, their storage, and efficient use, in accordance with the principles of a circular economy. The project was built on the research base of the National Center for Energy, integrated existing research capacities into the long-term strategic concept of CEET, and met the requirements of the State Energy Policy of the Czech Republic and the NAP. Without the unique merger and combination of the three logically linked research programmes, the desired synergy and rapid market feasibility would never have been achieved.

#### **Common Actuator Controller (2021–2022)**

- Project ID: CZ.01.1.02/0.0/0.0/20\_321/0024308
- Principal Investigator: Prof. Stanislav Mišák
- Grant Provider: MIT CR

→ The project focused on the research and development of a new generation of modular control units for advanced aviation electromechanical actuators, which will find use in the next generation of aviation platforms known as More Electric Aircraft (MEA) and in the next generations of Full Electric Aircraft (FEA). These should contribute to making air transport more environmentally friendly by significantly increasing the use of electricity, which entails several changes, including a switch to a substantially higher voltage on-board network.

# International Projects

## Supercomputing Services Projects

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

### PRACE-6IP – Partnership for Advanced Computing in Europe, 6<sup>th</sup> Implementation Phase (2019–2022)

- Project ID: 823767 (H2020 INFRAEDI-2018-2020)
- Principal Investigator: Doc. Vít Vondrák
- The project's objective was 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. Unlike the previous ones, the sixth project in a row to support the pan-European PRACE research infrastructure and its users was focused on the identification and development of new applications with significant potential to exploit the capacity of exascale supercomputers.  
→ [www.prace-ri.eu](http://www.prace-ri.eu)

### DICE – Data Infrastructure Capacity for EOSC (2021–2023)

- Project ID: 101017207 (H2020-INFRAEOSC-2018-2020, RIA)
- Principal Investigator: Filip Staněk
- The project consortium brings together a network of computing and data centres, research infrastructures, and data repositories to enable a European storage and data management infrastructure for EOSC, providing generic services and building blocks to store, find, access, and process data consistently and persistently.  
→ [www.dice-eosc.eu](http://www.dice-eosc.eu)

## Science and Research Projects

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

### EUROCC – National Competence Centres in the Framework of EuroHPC (2020–2022)

- Project ID: 951732 (H2020-JTI-EuroHPC-2019-2)
- Principal Investigator: Dr Tomáš Karásek
- The project brought 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. It aimed to strengthen expertise and skills in high-performance computing, data analytics, and artificial intelligence and to bridge the existing national gaps in using these technologies. → [www.eurocc-project.eu](http://www.eurocc-project.eu)

### POP2 – Performance Optimisation and Productivity 2 (2018–2022)

- Project ID: 824080 (H2020-INFRAEDI-2018-1)
- Principal Investigator: Doc. Lubomír Říha
- The POP2 Centre of Excellence built on the Performance Optimisation and Productivity 1 (POP1) project and extended its activities. The main aim of POP2 was to assist with the 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](http://www.pop-coe.eu)

### LIGATE – Ligand Generator and portable drug discovery platform AT Exascale (2021–2023)

- Project ID: 956137 (H2020-JTI-EuroHPC-2019-1, EuroHPC-IA)
- Principal Investigator: Dr Jan Martinovič
- The project aims to integrate and co-design best-in-class European open-source components together with proprietary IPs to keep worldwide leadership on Computer-Aided Drug Design (CADD) solutions exploiting today's high-end supercomputers and tomorrow's Exascale resources, fostering European competitiveness in this field. The proposed LIGATE solution, in a fully integrated workflow, enables to deliver the result of a drug design campaign with the highest speed and accuracy; further implementation of auto-tuning the parameters of the solutions to meet the time and resource constraints. → [www.ligateproject.eu](http://www.ligateproject.eu)

### EVEREST – dEsign enVironmEnt foR Extreme-Scale big data analytics on heterogeneous platforms (2020–2024)

- Project ID: 957269 (H2020-ICT-2018-20 / H2020-ICT-2020-1)
- Principal Investigator: Dr Kateřina Slaninová
- The project is developing a holistic approach for co-designing computation and communication in the high-tech and especially secure system for HPDA. This will be achieved by simplifying the programmability of heterogeneous and distributed architectures through a “data-driven” design approach, using hardware-accelerated AI, and the efficient monitoring of the execution with a unified hardware-software paradigm. The project will validate its approach by applying it in real-life business scenarios such as a weather analysis-based prediction model, an application for air-quality monitoring, and a smart city traffic modelling framework. → [www.everest-h2020.eu](http://www.everest-h2020.eu)

### ACROSS – HPC big data artificial intelligence cross stack platform towardS exaScale (2021–2024)

- Project ID: 955648 (H2020-JTI-EuroHPC-2019-1, EuroHPC-IA)
- Principal Investigator: Dr Jan Martinovič
- The project aims to co-design and develop an HPC, BD, and Artificial Intelligence (AI) convergent platform, supporting applications in the Aeronautics, Climate and Weather, and Energy domains. To this end, the project will leverage the next generation of pre-exascale infrastructures, still ready for exascale systems and effective mechanisms to easily describe and manage complex workflows in the three domains mentioned. The project combines traditional HPC techniques with AI (specifically machine learning/deep learning) and BD analytic techniques to enhance the application test case outcomes. → [www.acrossproject.eu](http://www.acrossproject.eu)

**s-NEBULA – Novel Spin-Based Building Blocks for Advanced TeraHertz Applications (2020–2024)**

- Project ID: 863155 (H2020-FETOPEN-2018-2020, RIA)
- Principal Investigator: Doc. Kamil Postava
- The project aims to research and develop a revolutionary approach to TeraHertz (THz) technology for generating and detecting THz radiation, initiating the new field of spin-based TeraHertz technology. The project aims to provide a platform of room-temperature innovative spin-based THz building blocks arising from novel combinations of magnetism and optics. The project will provide cutting-edge solutions to solve bottleneck scientific issues in the THz field motivated by clear needs in judiciously chosen target applications. → [www.s-nebula.eu](http://www.s-nebula.eu)

**SCALABLE – SCALable Lattice Boltzmann Leaps to Exascale (2021–2023)**

- Project ID: 956000 (H2020-JTI-EuroHPC-2019-1, EuroHPC-IA)
- Principal Investigator: Doc. Lubomír Říha
- The project brings together eminent industrial and academic partners to improve the performance, scalability, and energy efficiency of industrial Lattice Boltzmann methods-based computational fluid dynamics (CFD) software. The Lattice Boltzmann method (LBM) provides a reliable alternative to conventional CFD approaches. LBM is exceptionally well suited to exploit advanced supercomputer architectures as it enables massive parallelisation. The project will directly benefit European industry while contributing to fundamental research. → [www.scalable-hpc.eu](http://www.scalable-hpc.eu)

**IO-SEA – IO Software for Exascale Architecture (2021–2024)**

- Project ID: 955811 (H2020-JTI-EuroHPC-2019-1, EuroHPC-RIA)
- Principal Investigator: Dr Jan Martinovič
- IO-SEA aims to provide a novel data management and storage platform for exascale computing based on hierarchical storage management (HSM) and on-demand provisioning of storage services. The platform will efficiently use storage tiers spanning NVMe and NVRAM at the top all the way down to tape-based technologies. Advanced IO instrumentation and monitoring features will be developed within the project, leveraging the latest AI and machine learning advancements to systematically analyse the telemetry records and make smart decisions on data placement. → [www.iosea-project.eu](http://www.iosea-project.eu)

**OPENQKD – Open European Quantum Key Distribution Testbed (2019–2023)**

- Project ID: 857156 (H2020-SU-ICT-2018-2020)
- Principal Investigator: Prof. Miroslav Vozňák
- The project aims to establish a testbed for a highly secure network using the principles of quantum mechanics for key distribution. It has been the most extensive 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 PSNC (Poznan). The second is participation in the development and implementation of key management. The third is a simulation of the QKD use cases of all partners in the project and the improvement of an open/source QKD simulator, which is being developed as an open source. The computational resources of IT4Innovations are used for the simulations. → [www.openqkd.eu](http://www.openqkd.eu)

**EUPEX – European Pilot for Exascale (2022–2025)**

- Project ID: 101033975 (H2020-JTI-EuroHPC-2020-01, RIA)
- Principal Investigator: Doc. Lubomír Říha
- The EUPEX consortium aims to design, build, and validate the first EU platform for HPC, covering end-to-end the spectrum of required technologies with European assets: from the architecture, processor, system software, and development tools to the applications. The EUPEX prototype will be designed to be open, scalable, and flexible, including the modular OpenSequana-compliant platform and the corresponding HPC software ecosystem for the Modular Supercomputing Architecture. Scientifically, EUPEX is a vehicle to prepare HPC, AI, and Big Data processing communities for upcoming European Exascale systems and technologies. → [www.eupex.eu](http://www.eupex.eu)

**Projects of the 9<sup>th</sup> Framework Programme for Research and Innovations of the European Union – Horizon Europe**

**BioDT – Biodiversity Digital Twin for Advanced Modelling, Simulation and Prediction Capabilities (2022–2025)**

- Project ID: 101057437 (HORIZON-INFRA-2021-TECH-01, RIA)
- Principal Investigator: Dr Tomáš Martinovič
- BioDT aims to push the current boundaries of a predictive understanding of biodiversity dynamics by developing a Digital Twin providing advanced modelling, simulation, and prediction capabilities. By exploiting existing technologies and data available across relevant research infrastructures in new ways, the BioDT project will be able to model the interaction between species and their environment accurately. Scientists at Research Infrastructures will be able to use the BioDT to 1) better observe changes in biodiversity, 2) relate these changes to possible causes, and 3) better predict the effects of changes based on influences on these causes by either climate or human intervention. The consortium brings together a dynamic team of experts in biodiversity, high-performance computing, and artificial intelligence. → [www.biodt.eu](http://www.biodt.eu)

**OpenWebSearch.EU – Piloting a Cooperative Open Web Search Infrastructure to Support Europe’s Digital Sovereignty (2022–2025)**

- Project ID: 101070014 (HORIZON-CL4-2021-HUMAN-01, RIA)
- Principal Investigator: Dr Jan Martinovič
- In the OpenWebSearch.EU project, 14 renowned European research and supercomputing centres joined forces to develop an open European infrastructure for web search. This project will contribute to Europe’s digital sovereignty and promote an open human-centred search engine market. Within three years, the researchers will develop the core of a European Open Web Index as a basis for a new Internet Search in Europe. In addition, the project will set the foundation for an open and extensible European open Web Search and Analysis Infrastructure based on Europe’s values, principles, legislation, and standards. → [www.openwebsearch.eu](http://www.openwebsearch.eu)

## Educational Projects

### Erasmus+ projects

#### SCtrain – Supercomputing knowledge partnership (2020–2023)

- Project ID: 20-203-075975 (KA203-6E6A1FFC)
- Principal Investigator: Prof. Tomáš Kozubek
- The mission of this project is to use a methodical approach to fill gaps in current university courses and increase awareness of HPC for future professionals in science, technology, engineering, and mathematics. → <https://sctrain.eu/>

### Projects of the 8<sup>th</sup> Framework Programme for Research and Innovations of the European Union – Horizon 2020

#### EUMaster4HPC – European Master for High Performance Computing (2022–2025)

- Project ID: 101051997 (H2020-JTI-EuroHPC-2020-03, CSA)
- Principal Investigator: Prof. Tomáš Kozubek
- The consortium, led by the University of Luxembourg, includes universities, research and supercomputing centres, industrial partners, and other cooperating institutions. The consortium aims to launch master's degree programmes at eight European universities: the University of Luxembourg, Universitat Politècnica de Catalunya, Politecnico di Milano, Friedrich-Alexander-Universität Erlangen-Nürnberg, Sorbonne Université, Sofia University St. Kliment Ohridski, Università della Svizzera Italiana, and Kungliga Tekniska Högskolan. It is envisaged that the list of participating universities and institutions will be expanded in the future. This activity is part of the broader EuroHPC Joint Undertaking strategy to support the development of key competencies and education and training in HPC for the needs of European science and industry. → [eumaster4hpc.uni.lu](http://eumaster4hpc.uni.lu)



↔ Karolina

The fifth IT4Innovations supercomputer was put into operation in the summer of 2021 as part of EuroHPC JU, which finances the acquisition of supercomputers in other European countries. Karolina is currently the most powerful supercomputer in the Czech Republic and one of the five EuroHPC petascale supercomputers.

# List of Abbreviations

AI	Artificial Intelligence
ACROSS	HPC big data artificial intelligence cross stack platform toward exascale
BD	Big Data
BDVA	Big Data Value Association
BioDT	Biodiversity Digital Twin for Advanced Modelling, Simulation and Prediction Capabilities
CEET	Centre for Energy and Environmental Technologies
CloudiFacturing	Cloudification of Production Engineering for Predictive Digital Manufacturing
CT	Computed Tomography
DICE	Data Infrastructure Capacity for EOSC
DIH	Digital Innovation Hub
DIHnet EU	Digital Innovation Hub Networks
DOI	Digital Object Identifier
EOSC	European Open Science Cloud
ESA	European Space Agency
ETP4HPC	European Technology Platform for High-Performance Computing
EUDAT CDI	EUDAT Collaborative Data Infrastructure
EUMaster4HPC	European Master For High Performance Computing
EUPEX	EUropean Pilot for EXascale
EUROCC	National Competence Centres in the framework of EuroHPC
EuroHPC JU	The European High Performance Computing Joint Undertaking
EVEREST	design environment for Extreme-Scale big data analytics on heterogeneous platforms
EXA4MIND	EXtreme Analytics for MINing Data spaces
ExaQUte	Exascale Quantifications of Uncertainties for Technology and Science Simulation
EXPERTISE	Experiments and High-Performance Computing for Turbine Mechanical Integrity and Structural Dynamics in Europe
FP7	Seventh Framework Programme
FTE	Full-time equivalent
GA CR	Grant Agency of the Czech Republic
GPU	Graphics Processing Unit
H2020	Horizon 2020
HPC	High-Performance Computing
HPCSE	The High Performance Computing in Science and Engineering Conference
HPDA	High Performance Data Analytics
HW	Hardware
ICT	Information and communications technology
IF	Impact Factor
IO-SEA	IO Software for Exascale Architecture
IoT	Internet of Things
IRS	Integrated Rescue System
LEXIS	Large-scale Execution for Industry & Society
LIGATE	Ligand Generator and portable drug discovery platform AT Exascale
LUMI	Large Unified Modern Infrastructure
LUMI-Q	Large Unified Modern Infrastructure for Quantum Computing
MEYS CR	Ministry of Education, Youth and Sports of the Czech Republic
MI CR	Ministry of the Interior of the Czech Republic
MIT CR	Ministry of Industry and Trade of the Czech Republic
MPI	Message Passing Interface

MSR	Moravian-Silesian Region
NCE	National Centre for Energy
NVIDIA DLI	NVIDIA Deep Learning Institute
OAGC	Open Access Grant Competition
OPENQKD	Open European Quantum Key Distribution Testbed
POP2	Performance Optimisation and Productivity 2
PRACE	Partnership for Advanced Computing in Europe
PRACE-6IP	Partnership for Advanced Computing in Europe, 6 <sup>th</sup> Implementation Phase
PTC	PRACE Training Center
QKD	Quantum Key Distribution
R&D&I	Research, Development and Innovation
SC22	Supercomputing Conference 2022
SCALABLE	SCALable LAttice Boltzmann Leaps to Exascale
SCtrain	Supercomputing Knowledge Partnership
SMEs	Small and medium-sized enterprises
s-NEBULA	Novel Spin-Based Building Blocks for Advanced TeraHertz Applications
SW	Software
TA CR	Technology Agency of the Czech Republic
TETRAMAX	Technology Transfer via Multinational Application Experiments
VR	Virtual Reality
VSU-TUO	VSU – Technical University of Ostrava



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