

Review 2023

Empowering innovations
with supercomputers
and a quantum computer.

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Managing Director's Introduction

Dear friends and partners of IT4Innovations, I am very pleased to present our Review 2023 publication, in which we look back at our key achievements and milestones and the operational and economic results we achieved that year.

Let me start by summarising the latest developments in our infrastructure. Last year, we made a significant step forward in quantum computing. In June, we signed an agreement to acquire and operate a quantum computer of the international LUMI-Q consortium with the EuroHPC Joint Undertaking. This quantum computer will be installed directly at IT4Innovations, representing a significant opportunity to strengthen our research capacity and innovations in quantum technologies. In this context, the transformation of the Big Data Analysis Lab into a new research lab dedicated specifically to quantum computing has begun.

Complementary systems consisting of several hardware platforms were installed and put into operation for all e-INFRA CZ users in the data room. These systems provide access to emerging, non-traditional, and highly specialised hardware architectures. A significant milestone in 2023 was the full acceptance of the most powerful European LUMI supercomputer, installed in Kajaani, Finland, in the acquisition, construction, and operation of which the Czech Republic also participates through IT4Innovations. Thanks to our membership in the LUMI consortium, the Czech scientific community has access to the computational resources of this unique Euro-

pean and global supercomputing infrastructure. Finally, we completed the migration of our supercomputers to the new Slurm workload management system, which is nowadays the most widespread in the field of supercomputers and represents a user standard.

The year 2023 was also marked by notable scientific achievements. The EXA4MIND project, coordinated by IT4Innovations, was launched to create a unique software platform for processing extreme data. We became partners of the MaX and SPACE Centres of Excellence in materials research and astrophysics, respectively, and joined new EOSC CZ, AIOOPEN, and DTO-BioFlow projects. In total, we participated in 21 international projects. In June, we joined the iRODS consortium, which brings together research organisations, universities, private companies, and public institutions worldwide, ensuring the development and sustainability of the eponymous software for distributed data storage, transfer, and management. In May, we launched a project focused on experimental and theoretical studies of near-infrared emitting chiral carbon dot luminophores under the auspices of the Moravian-Silesian Region's "Global Experts" programme. I would also like to highlight the research projects of our colleagues, which were printed in major world journals – two in Nature Communications, and the cover page with the result of our research appeared in The Journal of Physical Chemistry C.

We are also intensively involved in creating favourable conditions for the uptake of supercomputers by small and medium-sized enterprises and start-ups. At the beginning of 2023, the European Digital Innovation Hub Ostrava started its activities to support introducing and using digital technologies, primarily in small and medium-sized enterprises and public organisations. The National Competence Centre in HPC, the services of which are provided by IT4Innovations in the Czech Republic, entered the second phase of its existence.

We are always proud of our colleagues' achievements. Pierre Koleják was awarded the Talent of the Year award, which the City of Ostrava gives to exceptional students. Radek Halfar received 1st place for his dissertation entitled Dynamics of Cardiac Electrophysiology Models in the Information Technology and Electrical Engineering category of the VSB-TUO competition and 7th place in the 2023 Werner von Siemens Award competition.

In conclusion, I would like to thank all the employees of IT4Innovations for their hard work and dedication, which has helped us achieve these excellent results. I would also like to thank our partners and supporters for their continued support. We look forward to another year of excellence, innovation, and success.



Vít Vondrák

Managing Director



↔ The IT4Innovations building was officially opened in 2014.

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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. 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 competitiveness and innovativeness of Czech science and industry. Together with the CESNET and CERIT-SC, 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 (MEYS).

IT4Innovations is currently operating two supercomputers: [Karolina](#) (15.7 PFlop/s, installed in the summer of 2021) and [Barbora](#) (849 TFlop/s, installed in the autumn of 2019), and also a specialised system for artificial intelligence computations [NVIDIA DGX-2](#) (2 PFlop/s for AI, installed in the spring of 2019). The very first supercomputers installed at IT4Innovations include Anselm (94 TFlop/s, installed in the summer of 2013) and Salomon (2 PFlop/s, installed in the summer of 2015), the operations of which were ceased in 2021. As a member of the LUMI consortium, IT4Innovations also participates in the operation of the [LUMI](#) supercomputer, the fifth most powerful supercomputer in the world and the most powerful supercomputer in Europe, located in Kajaani, Finland. As a result, the Czech research community also has access to this supercomputer (531.5 PFlop/s).

The IT4Innovations data room also houses [complementary systems](#) consisting of several hardware platforms. These systems provide users with access to emerging, non-traditional, and highly specialised hardware architectures.

In 2024, the first Czech [quantum computer](#) acquired within the European LUMI-Q consortium will also be installed at IT4Innovations. The quantum computer will be based on superconducting qubits in a star-shaped topology and will contain at least 20 qubits. It will be used by the entire user base of the EuroHPC JU.

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

IT4Innovations research activities were executed across five laboratories in 2023:

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

IT4Innovations is the [National Competence Centre in HPC](#), a member of the [MaX](#), [SPACE](#), and [POP3 Centres of Excellence](#) and a partner of [more than ten other international Horizon 2020](#), [Horizon Europe](#), and [Digital Europe projects](#), coordinating the [EXA4MIND](#) and [EDIH Ostrava](#) projects.

IT4Innovations has been highly active in collaboration with industry. In 2023, the [European Digital Innovation Hub Ostrava](#) (EDIH Ostrava), established by bringing together the activities of IT4Innovations, the Faculty of Electrical Engineering and Computer Science of VSB – Technical University of Ostrava, and the Moravian-Silesian Innovation Centre Ostrava, started its activities. The EDIH Ostrava is part of the European Digital Innovation Hubs network, which supports the deployment and use of digital technologies primarily in small and medium-sized enterprises to support their competitiveness.

IT4Innovations also offers a wide range of [specialised training courses](#) focused on HPC, HPDA, AI, QC, and acquiring the knowledge needed to use supercomputing infrastructure effectively. In the above fields, IT4Innovations is also involved in educating students, primarily within the [Computational and Applied Mathematics](#) MSc study programme and [Computational Sciences](#) and [Informatics and Computational Sciences](#) PhD study programmes offered by the Faculty of Electrical Engineering and Computer Science of VSB-TUO. In 2023, the first students at the same faculty studied a new course entitled [Introduction to Quantum Computing](#), which was prepared by IT4Innovations experts. IT4Innovations is also a member of the [EUMaster4HPC](#) consortium, which implements the eponymous pan-European MSc study programme focused on high-performance computing.

History

- 2011**
 - Foundation of IT4Innovations
 - Membership in PRACE (Partnership for Advanced Computing in Europe)
- 2013**
 - Launch of the Anselm supercomputer
- 2014**
 - Opening of the IT4Innovations building
- 2015**
 - Launch 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
- 2019**
 - Launch of the Barbora supercomputer and the specialised NVIDIA DGX-2 system
 - Membership in BDVA (Big Data Value Association) and EUDAT CDI
 - Foundation of e-INFRA CZ
 - Launch 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**
 - Launch 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
- 2023**
 - IT4Innovations becomes a member of the iRODS consortium
 - Completion of the complementary systems' installation
 - Launch of the EXA4MIND project, the coordinator of which is IT4Innovations
 - IT4Innovations becomes part of the MaX and SPACE Centres of Excellence

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 its 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 processing of advanced data sets for the benefit of science, industry, and society.

Memberships 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
- LUMI-Q – Large Unified Modern Infrastructure for Quantum Computing
- iRODS – Integrated Rule-Oriented Data System
- PRACE – Partnership for Advanced Computing in Europe

Organisational Structure

Organisational Structure of IT4Innovations



Scientific Council of IT4Innovations

Chairman | 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 2023, the number of IT4Innovations employees converted to full-time equivalents (FTEs) totalled 159.32 FTEs, which consists of:

25.7% Management and Administration

12.1% Supercomputing Services

62.2% Research and Development:

- 43.2% Advanced Data Analysis and Simulations Lab
- 16.4% Modelling for Nanotechnologies Lab
- 14.9% Infrastructure Research Lab
- 22.5% Parallel Algorithms Research Lab
- 3.0% Big Data Analysis Lab



KAROLINA

↔ In 2023, IT4Innovations operated two supercomputers, Karolina and Barbora.

2

Important Events

January

→ The Launch of the three-year **EuroCC 2** project ensures the continuation of the **National Competence Centre in HPC (NCC)**, represented by IT4Innovations. The NCC primarily aims to offer a broad portfolio of HPC services, promote European cooperation, and strengthen Czech companies' technological independence and competitiveness.

→ The cover of **The Journal of Physical Chemistry B** is adorned with an image of lipid nanoparticle research by CATRIN and IT4Innovations scientists.

→ Michal Otyepka participated in **developing a new nanomaterial** that instantly detects antibiotics in water.

→ IT4Innovations is a member of the **SPACE** (Scalable Parallel Astrophysical Codes for Exascale) **European Centre of Excellence**, which aims to prepare applications used in astrophysics and cosmology research for the exascale era.

→ The EXA4MIND project, coordinated by IT4Innovations, was launched to create an extreme data platform combining data storage facilities and supercomputers.

→ IT4Innovations became a partner of the **MaX (MAterials design at the eXascale) Centre of Excellence** to enable modelling, simulations, and discovery and design of materials at the interface of current and future high-performance computing (HPC) and data analytics technologies.

→ The **European Digital Innovation Hub Ostrava** launched its activities. It aims to support introducing and using digital technologies, primarily in small and medium-sized enterprises and public organisations.

→ The **EOSC-CZ** (European Open Science Cloud) project, which will connect existing scientific communities and create a platform for systematic work and data storage and sharing, launched its activities in the Czech Republic. This will make it easier and faster for scientists and scientific organisations to access research data.

February

→ **LUMI**, Europe's most powerful supercomputer, was fully accepted. The Czech scientific community can apply for computational resources on LUMI within open access grant competitions, which IT4Innovations announces three times a year, completely free of charge. LUMI is installed in Kajaani, Finland.

March

→ Jan Martinovič received an **award for the EXA4MIND** project at a formal meeting of the Scientific Board of VSB-TUO.

April

→ Scientists from IT4Innovations developed a **unique technology** that will allow the waste from biodiesel production to be used and converted into valuable products, thus increasing the efficiency of existing biofuels. The research results were published in the Nature Communications journal.

May

→ Launch of the Experimental and theoretical studies of near-infrared emitting chiral carbon dot luminophores project under the auspices of the Moravian-Silesian Region's **Global Experts** programme. The programme aims to attract world-leading scientists to universities in the Moravian-Silesian Region. Professor Andrey Rogach joins IT4Innovations.

→ The latest research results of the **Cell Tracking Challenge**, in which IT4Innovations is involved, were published in the prestigious Nature Methods journal.

→ The international LUMI-Q consortium and the EuroHPC Joint Undertaking signed an agreement to acquire and operate a quantum computer, which will be installed at IT4Innovations.

→ IT4Innovations became a member of the [iRODS consortium](#). The consortium brings together enterprises, research organisations, universities, and governmental organisations worldwide to ensure the sustainability of iRODS (Integrated Rule-Oriented Data System) software as a solution for distributed storage, transfer, and management of data.

→ The voicebot, developed by researchers from IT4Innovations and activated when emergency lines are extremely overloaded, won the award of the European [DT4REGIONS](#) initiative promoting the use of AI in public administration for the most innovative solution.

→ Our colleague Pierre Koleják won the [Talent of the Year](#) award given by the city of Ostrava to exceptional students.

→ The bachelor thesis “Visualisation of Traffic Flow Evolution Over Time” by Pavlína Smolková under the supervision of Kateřina Slaninová from IT4Innovations won the [award for excellent quality](#). The thesis focuses on creating a video showing the direction and intensity of traffic in individual sections of the traffic network.

→ The cover of [The Journal of Physical Chemistry C](#) is adorned with an image from a research project describing the formation of amide bonds on the surface of graphene, in which scientists from CATRIN, the Czech Academy of Sciences, Technische Universität Dresden, Technische Universität München, Indian Institute of Technology – Jammu, and VSB-TUO collaborated.

→ The collaborative research of the Czech Academy of Sciences, Palacký University Olomouc, and IT4Innovations was published in [Nature Communications](#). The scientists worked on visualising π -holes in molecules using Kelvin probe force microscopy, for which they also used IT4Innovations supercomputers. The research authors include Professor Pavel Hobza and Maximilian Lamanec from IT4Innovations.

→ The European Space Agency (ESA) supported the [AIOPEN](#) project. During the project, two case studies will be carried out on the platform, with IT4Innovations responsible for the Urban Change Detection with Transformer Architecture case study.

→ The [DTO-BioFLOW](#) project (Integration of biodiversity monitoring data into the Digital Twin Ocean) was launched. The project involves 30 partners, including IT4Innovations.

→ Migration to the new Slurm workload management system for supercomputers completed.

→ Jiří Tomčala received the [Quantum Excellence](#) certificate awarded by IBM.

→ A new “green” way to [produce hematene](#), a two-dimensional material derived from the iron mineral hematite with great potential for use in clean energy and environmental applications, was found by researchers from Palacký University and VSB-TUO in a paper published in [Applied Materials Today](#). The research, which was co-authored by Michal Otyepka of IT4Innovations, made the journal's cover.

→ Nearly 700 visitors discovered the secrets of supercomputers at IT4Innovations thanks to the pan-European [Researchers' Night](#) event.

→ The continuation of the [Superheroes 4 Science project](#), which is committed to introducing the younger generation to the fascinating world of high-performance and quantum computing, was launched. The project is supported by the Czech Republic, Poland, and Slovakia governments through the International Visegrad Fund.

→ The publication “[Scalable Algorithms for Contact Problems](#)”, authored by Zdeněk Dostál, Tomáš Kozubek, Marie Sadowská, and Vít Vondrák, with contributions by Tomáš Brzobohatý, Lubomír Říha, Oldřich Vlach, and David Horák, was released.

→ At the 7th [Users' Conference of IT4Innovations](#), we welcomed almost 90 participants.

→ In cooperation with IXPERTA, [a software simulator of railway track conditions was developed](#) to create a functional sample of a detection system for railway safety.

3

Financial Review

IT4Innovations Economic Balance

The total expenditures of IT4Innovations amounted to **CZK 305,486,000** in 2023. Of this amount, operating (non-investment) and investment (capital) expenditures accounted for 90.1% and 9.9%, respectively.

Operational expenditures amounted to CZK 275 million in 2023. The most significant part of these expenditures consisted of personnel costs, services (electricity consumption costs, maintenance of operated computing and data systems and supporting infrastructure, technical and system support, etc.), and overheads.

Investment expenditures in 2023 amounted to CZK 30 million. They included, among other things, the extension of the PROJECT data storage, the acquisition of complementary systems II, and the modernisation of meeting rooms.

Profit before tax in 2023 amounted to CZK 3,420,000.

Economic balance of IT4Innovations

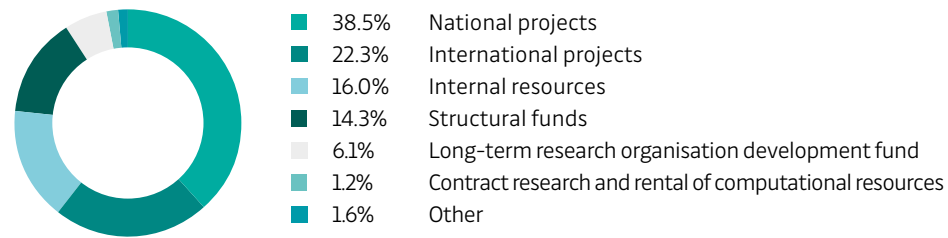
A. Total operational expenditures	CZK 275,297,000
Personnel costs – research teams	CZK 98,084,000
Personnel costs – management and administration	CZK 40,913,000
Personnel costs – supercomputing services	CZK 20,017,000
Services	CZK 63,472,000
Overheads	CZK 37,489,000
International and domestic business trips (incl. invited lecturers)	CZK 7,443,000
Small fixed assets	CZK 2,334,000
Consumables	CZK 2,195,000
Fees	CZK 2,246,000
Other costs	CZK 782,000
Scholarships	CZK 322,000
B. Total investment expenditures	CZK 30,189,000
Tangible fixed assets – machines and equipment	CZK 28,674,000
Tangible fixed assets – buildings	CZK 1,515,000
C. Total expenditures (A+B)	CZK 305,486,000
D. Total sources of funding	CZK 308,906,000
E. Balance total (D-C)	CZK 3,420,000

Sources of Funding

In 2023, IT4Innovations' overall budget was CZK 308,906,000. National projects accounted for the largest share of funding sources, followed by international projects. The other most crucial funding sources for IT4Innovations were internal resources (operating fund, contribution to educational activities) and structural funds.

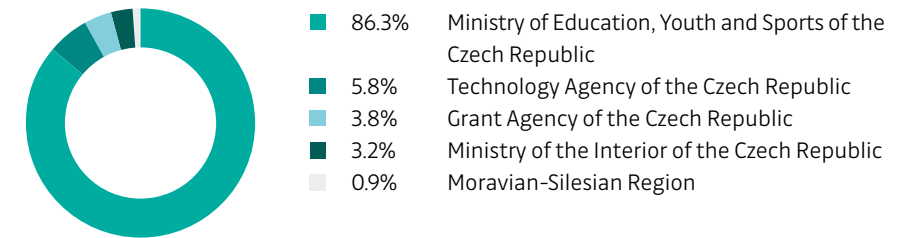
Sources of funding for the institute's costs

CZK 308,906,000 in total



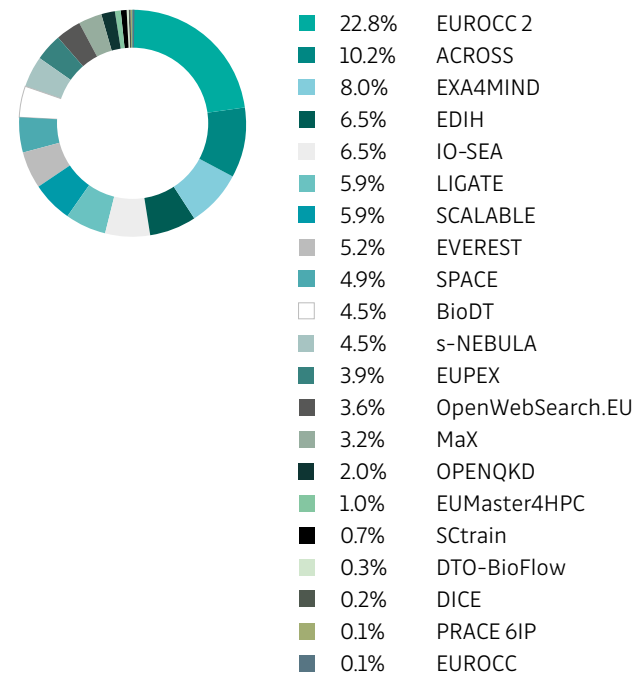
National projects

CZK 118,762,000 in total



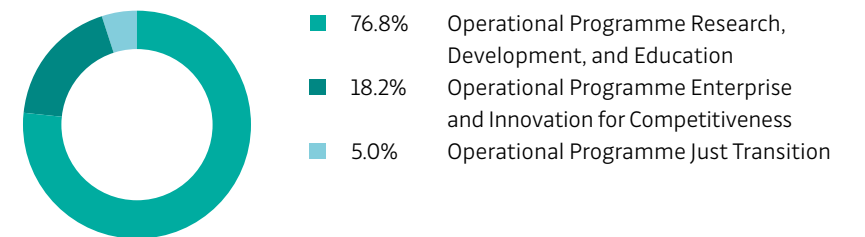
International projects

CZK 68,957,000 in total



European structural and investment funds

CZK 44,166,000 in total



List of Projects

National projects

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

Large Infrastructure for Research, Experimental Development and Innovation Project

- e-Infrastructure CZ
- e-INFRA CZ: Modernisation

Projects of the Operational Programme Johannes Amos Comenius

- e-INFRA CZ Modernisation II
- European Open Science Cloud Czech Republic

Projects of the Operational Programme Research, Development and Education

- Artificial Intelligence and Reasoning
- 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

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)

Global Experts programme

- Experimental and theoretical studies of near-infrared emitting chiral carbon dot luminophores project

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

International Grant Projects Evaluated on the LEAD Agency principle

- Magnetism at interfaces: from quantum to reality

Standard Grant Projects

- Unconventional superconductors under extreme conditions
- Novel thermoelectric, thermovoltaic, and phonoelectric heat conversion systems based on nitrides semiconductors

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

TREND Programme

- Combination of Holographic and Digital Safety Protection

ÉTA Programme

- Creating a model for evaluating the impact of changes 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

- SmartFleet – AI based software for 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 for digital transformation

Projects of the Operational Programme Technologies and Application for Competitiveness

- Terahertz Raman spectrometers with enhanced application capabilities

Projects supported by the Ministry of the Interior of the Czech Republic (MI CR)

- Research on Holistic Model of Interconnected Critical Electricity and Communication Infrastructures

VSB-TUO Projects with IT4Innovations Participation

- Energy System for Grids
- REFRESH – Research Excellence For REgion Sustainability and High-tech Industries
- Validation of integrating artificial intelligence for receiving emergency calls

International projects

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

- ACROSS – HPC big data artificial intelligence cross stack platform toward exascale
- DICE – Data Infrastructure Capacity for EOSC
- EUMaster4HPC – European Master for High-Performance Computing
- EUPEX – European Pilot for EXascale
- EVEREST – Design Environment for Extreme-Scale big data analytics on heterogeneous platforms
- IO-SEA – IO Software for Exascale Architecture
- LIGATE – Ligand Generator and portable drug discovery platform AT Exascale
- OPENQKD – Open European Quantum Key Distribution Testbed
- s-NEBULA – Novel Spin-Based Building Blocks for Advanced Terahertz Applications
- SCALABLE – Scalable Lattice Boltzmann Leaps to Exascale

Projects of the 9th Framework Programme for Research and Innovation of the European Union – Horizon Europe

- BioDT – Biodiversity Digital Twin for Advanced Modelling, Simulation and Prediction Capabilities
- DTO-BioFlow – Integration of biodiversity monitoring data into the Digital Twin Ocean
- EXA4MIND – Extreme Analytics for MINing Data spaces
- MaX – Materials design at the exascale
- OpenWebSearch.EU – Piloting a Cooperative Open Web Search Infrastructure to Support Europe's Digital Sovereignty
- SPACE – Scalable Parallel and distributed Astrophysical Codes for Exascale

Digital Europe Programme

- EUROCC 2 – National Competence Centres in the Framework of EuroHPC Phase 2
- EDIH Ostrava – European Digital Innovation Hub Ostrava
- CZQCI – Czech National Quantum Communication Infrastructure

Erasmus+ Projects

- Sctrain – Supercomputing knowledge partnership

International Visegrad Fund

- Superheroes 4 Science

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.

Supercomputers

In 2023, IT4Innovations operated two supercomputers – **Karolina** (15.7 PFlop/s) and **Barbora** (849 TFlop/s), and the specialised system for artificial intelligence computations **NVIDIA DGX-2** (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 JU membership countries. Immediately after its launch, it ranked among the most powerful supercomputers in Europe – in the TOP500 list, which evaluates supercomputers in terms of their performance, it ranked 69th in Europe. In the Green500 list of the most energy-efficient supercomputers, Karolina ranked 8th globally and 3rd in Europe.

Since 2023, the **LUMI** supercomputer has been fully operational, with its theoretical peak performance of 531.5 PFlop/s. Thanks to IT4Innovations' membership in the LUMI (Large Unified Modern Infrastructure) consortium of eleven 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), participates in its operation, and develops software tools such as HyperQueue, which enables users to use the available LUMI's computational resources effectively.

In 2023, when the LUMI supercomputer was made fully operational and accepted, 101 scientific projects were awarded LUMI computational resources through the IT4Innovations calls, totalling almost 1 million node hours.

We rely on the concept of node hours to evaluate the utilisation of IT4Innovations computational resources, since computer clusters and individual nodes have different architectures and performance. Each computing system has specific parameters such as processor types, graphics accelerators, and other factors that affect its performance. Although we aggregate these node hours on computer clusters in the following text for the sake of simplicity, they do not reflect the different performance of individual compute nodes.

Complementary systems

The latest addition to IT4Innovations is **complementary systems** consisting of several hardware platforms. These systems provide access to emerging, non-traditional, and highly specialised hardware architectures. The first part was put into operation in IT4Innovations in the autumn of 2022, and in 2023, other hardware platforms were delivered. IT4Innovations offers the users of its computational resources, especially software developers, the opportunity to test their applications on hardware they may encounter in other computing centres (e.g. EuroHPC LUMI or Deucalion systems) or upcoming systems, both national and foreign (e.g. JUPITER).

PROJECT data storage

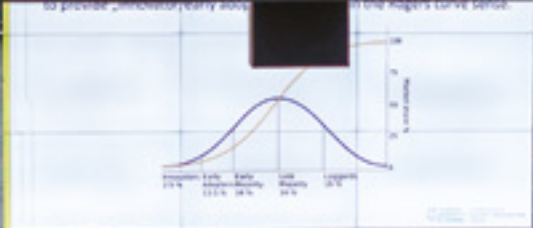
IT4Innovations data room also houses the **large-capacity PROJECT data storage**, which saves and backs up data processed or generated on the IT4Innovations supercomputers. The PROJECT data storage is a central storage for both IT4Innovations project and user data. A project directory is created for every active project, and it strictly follows the project's life cycle. The total capacity of the storage is 15 PB.

Quantum computer

In 2023, IT4Innovations signed an agreement with the EuroHPC JU to acquire and operate the international **LUMI-Q** consortium's **quantum computer**, which will be installed and operated at IT4Innovations. The quantum computer will be based on superconducting qubits in a star-shaped topology that minimises the number of so-called swap operations, enabling the implementation of highly complex quantum algorithms. The quantum computer will contain at least 20 qubits. It will also be connected to the Karolina supercomputer and become the first Czech quantum computer. The LUMI-Q quantum computer will be available to a wide range of European users, from the scientific community to industry and the public sector. The forthcoming quantum computing infrastructure will support the development of a wide range of industrial, scientific, and societal applications relevant to Europe. It will extend the European computing infrastructure with new technologies.

Technical Specifications of the Supercomputers

	NVIDIA DGX-2	Barbora	Karolina	LUMI
Put into operation	Spring 2019	Autumn 2019	Summer 2021	Winter 2023
Theoretical peak performance	130 TFlop/s	849 TFlop/s	15.7 PFlop/s	531.5 PFlop/s
Operating system	CentOS 7	RHEL 8	Rocky Linux 8.x	HPE Cray OS
Compute nodes	1	201	831	5,042
Types of compute nodes	<p>1 GPU node 2x Intel Xeon Platinum 8168, 24 cores, 2.7 GHz, 1.5 TB RAM, 16x NVIDIA Tesla V100, 32 GB HBM2</p>	<p>192 CPU nodes 2x Intel Cascade Lake 6240, 18 cores, 2.6 GHz, 192 GB RAM</p> <p>8 GPU nodes 2x Intel Skylake 6126, 12 cores, 2.6 GHz, 192 GB RAM, 4x NVIDIA Tesla V100, 16 GB HBM2</p> <p>1 SMP node 8x Intel Xeon 8153, 16 cores, 2.0 GHz, 6 TB RAM</p>	<p>756 CPU nodes 2x AMD EPYC 7h12, 64 cores, 2.6 GHz, 256 GB RAM (of which 36 nodes used for Cloud services)</p> <p>72 GPU nodes 2x AMD EPYC 7763, 64 cores, 2.45 GHz, 1 TB RAM, 8x NVIDIA A100, 40 GB HBM2</p> <p>1 data analytics node 32x Intel Xeon-SC 8628, 24 cores, 2.9 GHz, 24 TB RAM</p> <p>2 visualisation nodes 2x AMD EPYC 7452, 32 cores, 2.35 GHz, 256 GB RAM, 1x NVIDIA RTX 6000 GPU</p>	<p>2,048 CPU nodes 2x AMD EPYC 7763, 64 cores, 2.45 GHz, 256 – 1,024 GB RAM</p> <p>2,978 GPU nodes 1x AMD EPYC 7A53, 64 cores, 2.45 GHz, 512 GB RAM, 4x AMD Instinct MI250X GPUs, 128 GB HBM2e</p> <p>8 data analytics nodes 2x AMD EPYC 7742, 64 cores, 2.25 GHz, 4 TB RAM</p> <p>8 visualisation nodes 2x AMD EPYC 7742, 64 cores, 2.25 GHz, 2 TB RAM, 8x NVIDIA A40 GPU</p>
Accelerators in total	16x NVIDIA Tesla V100	32x NVIDIA Tesla V100	576x NVIDIA Tesla A100, 2x NVIDIA RTX 6000	11,912x AMD Instinct MI250X, 8x NVIDIA A40
CPU cores in total	48	7,232	106,880	454,784
Storage	30 TB NVMe	29 TB / home 310 TB / scratch (28 GB/s)	30 TB / home 1,275 TB / scratch (NVMe, 730 GB/s SWP, 1,198 GB/s SRP)	81 PB / (home + project + scratch) (240 GB/s)
Interconnection	Infiniband EDR 100 Gb/s	Infiniband HDR 200 Gb/s	Infiniband HDR 200 Gb/s	200 Gb/s Slingshot-11



↔ The 7th Users' Conference of IT4Innovations took place at the end of October.

Computational Resource Allocation

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

In June 2023, new rules for allocating HPC resources came into force. These bring new features or rename established types of computational resource allocation on our systems. Computational resources of IT4Innovations' supercomputers can be acquired in one of the following ways:

- **Open Access:** defines the allocation of computational resources to the research community in the Czech Republic based on scientific excellence, computing competence and readiness, and expected benefits for society and the economy. Computational resources are allocated on an open-access basis, with the aim of making HPC resources available for non-economic research and development activities. Eligible applicants are research organisations located in the Czech Republic or their employees. The largest share of computational resources is allocated through Open Access Grant Competitions.
- **Access to Thematic HPC Resource Utilisation:** computational resources are allocated for socially important tasks, teaching and educational activities, commercial activities, and in-house infrastructure research. Applications can be submitted anytime.
- **Grant Competitions**, which are announced by the EuroHPC JU.

From 2013 to the end of 2023, **2,174** projects from various scientific fields used computing time in IT4Innovations. These projects spanned a wide range of disciplines, including new materials and drug development, engineering tasks, and scientific data visualisation. In recent years, projects have increasingly focused on areas such as machine learning and other advanced technologies in the context of the development of artificial intelligence and research into quantum algorithms.

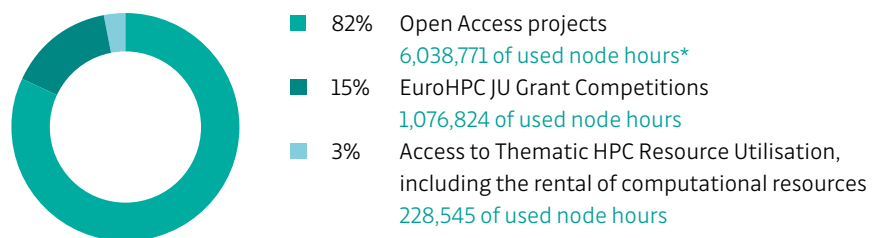
In 2023, **629** active projects were awarded computational resources, totalling **7,344,140** node hours.



↔ [Barbora](#)

The Barbora supercomputer was put into operation in 2019. Barbora refers to the saint patron of miners and was named after one of the mines located in the Ostrava-Karviná coal district.

Distribution of computational resources in 2023



*The node hours give an idea of the computational resources used in 2023. The total value here consists of all projects calculated at IT4Innovations using the Karolina and Barbora supercomputers and the NVIDIA DGX-2 system.

In the case of the LUMI supercomputer, 101 projects were allocated computational resources within the open access scheme, consuming almost half a million node hours by the end of 2023.

Open Access / Open Access Grant Competitions

In 2023, three Open Access Grant Competitions and one Special Call were announced, supporting 221 research projects, 23 of which were multi-year ones. Specifically, these were the 27th, 28th, and 29th calls and one special call dedicated to the AI community.

According to the schedule of each call, successful applicants were granted access to computational resources during 2023. For standard projects, computational resources are provided for 12 months. Multi-year projects have a duration of 24 or 36 months and are intended to support long-term research projects.

In these three Open Access Grant Competitions (and one special call), users applied for almost 10 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. In total, 8.7 million node hours available on the Karolina, Barbora, and LUMI supercomputers and the NVIDIA DGX-2 system were distributed across 221 projects in these calls of the Open Access Grant Competition.

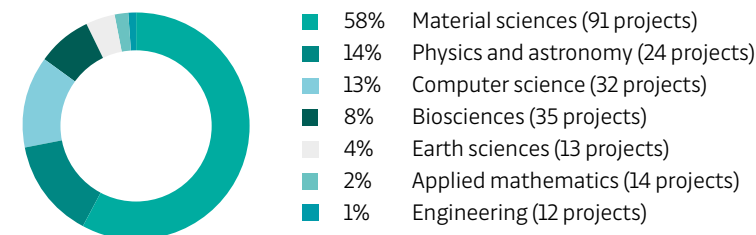
Projects in the field of material sciences received the most computational resources. The second place was taken by physics and astronomy projects, and computer science projects took the third place.

By institution, scientists from the Czech Academy of Sciences have received the highest allocations for their projects. The second and the third place belong to VSB – Technical University of Ostrava and Brno University of Technology, respectively.

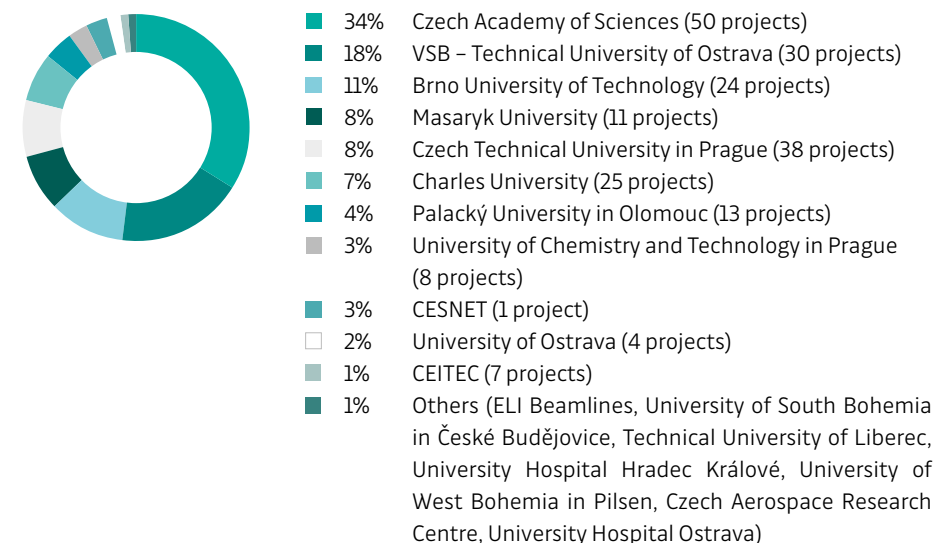
Most of the projects that received computational resources were submitted by scientists from the Czech Academy of Sciences, Czech Technical University in Prague, and VSB-TUO.

Investigators from 12 different institutes of the Czech Academy of Sciences received computational resources for a total of 50 projects. Among the institutes using the IT4Innovations infrastructure most were the Institute of Organic Chemistry and Biochemistry, the Institute of Physics, the J. Heyrovský Institute of Physical Chemistry, and the Institute of Physics of Materials, as in 2022.

Computational resources allocated within the Open Access Grant Competitions in 2023 by scientific discipline



Computational resources allocated within the Open Access Grant Competitions in 2023 by institutions



Open Access

The computational resources consumed within the Open Access Grant Competitions, including one special call, amounted to 6,032,073 node hours. Within the Fast Track Access, the primary objective of which is to prepare for the Open Access Grant Competitions, 6,638 node hours were consumed.

Access to thematic HPC resource utilisation

In 2023, 161,250 node hours were used for socially important tasks, teaching and educational activities, and in-house infrastructure research.

The computational resources provided within the paid rental amounted to 67,295 node hours. These were commercial projects of the following companies: AIRMOBIS s.r.o., DHI A/S, GLASS SERVICE, a.s., mobisOne s.r.o., and Varroc Lighting Systems, s.r.o.

At the beginning of December 2023, 115,007 node hours of LUMI-G were allocated within a special call for nine projects in artificial intelligence, mainly from the Czech Technical University in Prague and the Technical University of Liberec. This call was for socially important tasks: access to AI applications and GPU-accelerated applications to support the use of AI.

EuroHPC JU Grant Competitions

In 2023, 1,076,824 node hours of the Karolina supercomputer were allocated in these competitions, shared by 153 projects. Most of the projects were from organisations in Austria (e.g. Johannes Kepler University Linz – 15 projects), Italy (e.g. Politecnico di Milano – 3 projects), and Denmark (e.g. the University of Copenhagen and Technical University of Denmark – 8 projects).



- 25 projects Austria
- 24 projects Italy
- 18 projects Denmark
- 14 projects France
- 11 projects Spain
- 9 projects Germany
- 9 projects Sweden
- 7 projects Czech Republic
- 7 projects Turkey
- 4 projects Belgium
- 4 projects Romania
- 3 projects Great Britain
- 18 projects others (Israel, Portugal, Ireland, Norway, Greece, Switzerland, the Netherlands, Finland, Slovenia, Hungary, Poland, Luxembourg)

Users of computational resources

The number of active users of the IT4Innovations computing infrastructure increased by 48% year-on-year to 2,090 in 2023.

The IT4Innovations Technical Support provided to its users received 1,598 queries and requests in 2023. The internal response time (24 hours for the first response) was met for 98.4% of the queries. The internal closure time, which should not exceed 30 days, was met for 90% of the queries.



5

Research and Development

IT4Innovations conducts 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.

IT4Innovations is a research and development centre with strong international links. As such, it actively participates in all activities of the EuroHPC Joint Undertaking and several key international infrastructures, initiatives, and associations (PRACE, ETP4HPC, EUDAT, BDVA, EOSC, iRODS).

In 2023, IT4Innovations participated in implementing **21 international projects** funded by Horizon 2020, Horizon Europe, and Digital Europe, coordinating the EXA4MIND and EDIH Ostrava projects. It also became a member of the MaX and SPACE Centres of Excellence.

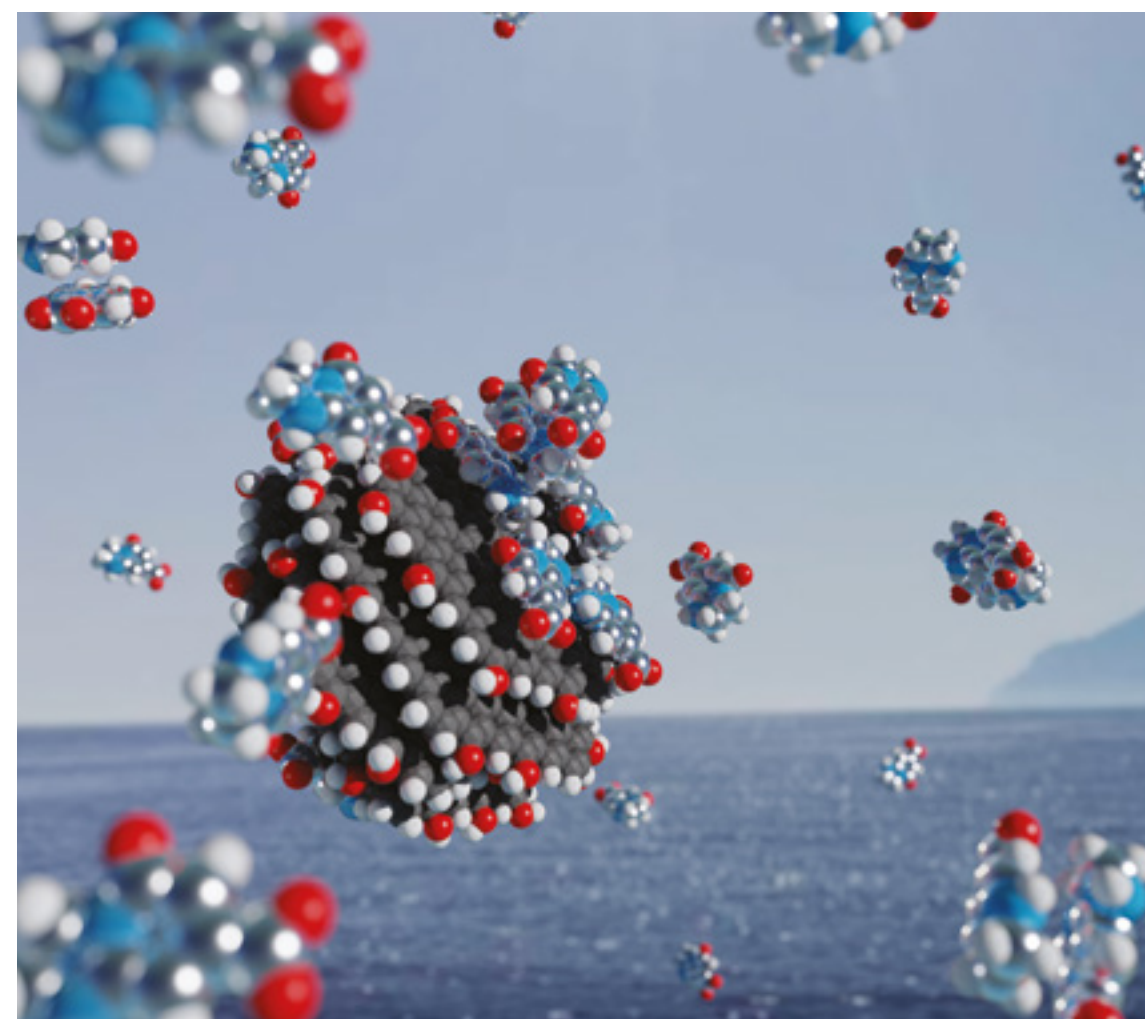
Since 2020, IT4Innovations has been the National Competence Centre in HPC within the European EuroCC project. The second phase of this project, EuroCC 2, started in 2023.

Since 2015, IT4Innovations has also been collaborating with the European Space Agency, and in 2023, it started the new AIOPEN (Platform Extensions with AI Capabilities) project with four partners.

IT4Innovations' research activities were carried out across five laboratories:

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

In 2023, IT4Innovations research labs were awarded nearly **1.47 million node hours** within the 27th to 29th Open Access Grant Competitions for implementing **21 research projects**, representing almost 17% of the total allocation of all supported projects. Most of the projects were submitted by researchers from the Advanced Data Analysis and Simulations Lab, and most computational resources were awarded to the Modelling for Nanotechnologies Lab.



↔ The Experimental and theoretical studies of near-infrared emitting chiral carbon dot luminophores project was launched

The project is supported by the Moravian-Silesian Region Global Experts programme.

Summary of Research and Development Results in 2023

Research and development results in 2023 based on the RIV 2017+ Methodology

This subsection presents the results of IT4Innovations research and development in 2023.

Summary of the achieved IT4Innovations research and development results in 2023

Results classified based on the RIV 2017+ Methodology	Achieved results
Jimp	118
JSC	5
Jost	0
B – reviewed publication	1
C – chapter in a reviewed publication	0
D – section in a proceeding	22
P – patent	1
F – utility model, industrial design	0
Z – semi-operation, verified technology	1
G – prototype, functional sample	0
H – results reflected in norms and directives	0
N – methodology, specialised map	0
R – software	27
V – research report	8

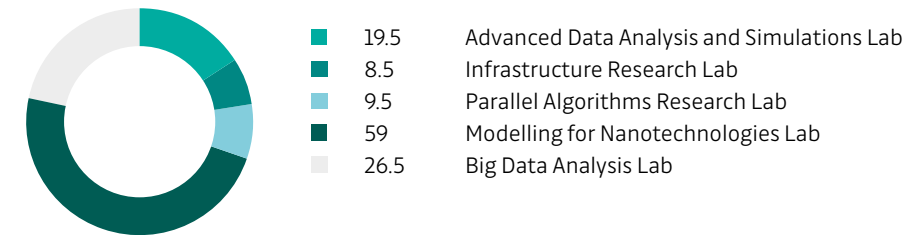
Jimp and JSC Journal Publications in 2023 by individual labs and ranking

Results based on the RIV 2017+ Methodology	D1	Q1/D1	Q2	Q3	Q4	Total
Advanced Data Analysis and Simulations Lab	12.5*	4	3	0	0	19.5
Infrastructure Research Lab	2.5*	3	2	1	0	8.5
Parallel Algorithms Research Lab	2	4	2.5*	1	0	9.5
Modelling for Nanotechnologies Lab	33.5*	17	6.5*	1	1	59
Big Data Analysis Lab	11.5*	12	3	0	0	26.5
Total	62	40	17	3	1	123

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

*Articles shared among labs

Number of journal publications in 2023 by individual labs



List of D1 publications sorted by individual labs

Advanced Data Analysis and Simulations Lab

→ Vavra O., Beránek J., Stourac J., Šurkovský M., Filipovic J., Damborsky J., Martinovič J., Bednar D.: *pyCaverDock: Python implementation of the popular tool for analysis of ligand transport with advanced caching and batch calculation support*. Bioinformatics, 2023. DOI 10.1093/bioinformatics/btad443. (D1, IF 5.8)

→ Lampart M., Zapoměl J.: *The disturbance influence on vibration of a belt device driven by a crank mechanism*. Chaos, Solitons & Fractals, 2023. DOI 10.1016/j.chaos.2023.113634. (D1, IF 7.8)

→ Maška M., Ulman V., Delgado-Rodriguez P., Gómez-de-Mariscal E., Nečasová T., Guerrero Peña Fidel A., Ren Tsang Ing, Meyerowitz Elliot M., Scherr T., Löffler K., Mikut R., Guo T., Wang Y., Allebach Jan P., Bao R., Al-Shakarji Noor M., Rahmon G., Toubal Imad E., Palaniappan K., Lux F., Matula P., Sugawara K., Magnusson Klass E.G., Aho L., Cohen Andrew R., Arbelle A., Ben-Haim T., Raviv Tammy R., Isensee F., Jäger Paul F., Maier-Hein Klaus H., Yanming Z., Ederra C., Urbiola A., Meijering E., Cunha A., Muñoz-Barrutia A., Kozubek M., Ortiz-de-Solórzano C.: *The Cell Tracking Challenge: 10 years of objective benchmarking*. Nature Methods, 2023. DOI 10.1038/s41592-023-01879-y. (D1, IF 48)

→ Klein L., Fulneček J., Seidl D., Prokop L., Mišák S., Dvorský J., Piecha M.: *A Data Set of Signals from an Antenna for Detection of Partial Discharges in Overhead Insulated Power Line*. Scientific data, 2023. DOI 10.1038/s41597-023-02451-1. (D1, IF 9.8)

→ Lampart M., Lampartová A., Orlando G.: *On risk and market sentiments driving financial share price dynamics*. Nonlinear Dynamics, 2023. DOI 10.1007/s11071-023-08702-5. (D1, IF 5.6)

→ Klein L., Seidl D., Fulneček J., Prokop L., Mišák S., Dvorský J.: *Antenna contactless partial discharges detection in covered conductors using ensemble stacking neural networks*. Expert Systems with Applications, 2023. DOI 10.1016/j.eswa.2022.118910. (D1, IF 8.5)

→ Zelinka I., Koječský L., Lampart M., Nowaková J., Plucar J.: *iSOMA swarm intelligence algorithm in synthesis of quantum computing circuits*. Applied Soft Computing, 2023. DOI 10.1016/j.asoc.2023.110350. (D1, IF 8.5)

- Riaz M. B., Jhangeer A., Martinovič J., Kazmi Syeda S.: *Dynamics and Soliton Propagation in a Modified Oskolkov Equation: Phase Plot Insights*. Symmetry, 2023. DOI 10.3390/sym15122171. (D1, IF 2.7)
- Halfar Radek, Lawson B.A.J., Weber dos Santos Rodrigo, Burrage K.: *Recurrence quantification analysis for fine-scale characterisation of arrhythmic patterns in cardiac tissue*. Scientific Reports, 2023. DOI 10.1038/s41598-023-38256-w. (D1, IF 4.6)
- Topolánek D., Krčál V., Foltyn L., Praks P., Vysocký J., Praksová R., Prettico G., Fulli G.: *Optimization method for short circuit current reduction in extensive meshed LV network*. International Journal of Electrical Power & Energy Systems, 2023. DOI 10.1016/j.ijepes.2023.109203. (D1, IF 5.2)
- Zahra A., Mardan S. A., Riaz M. B.: *Conformal motion for higher-dimensional compact objects*. European Physical Journal C, 2023. DOI 10.1140/epjc/s10052-023-12289-x. (D1, IF 4.4)
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- Marchamalo-Sacristán M., Ruiz-Armenteros A.M., Lamas-Fernández F., González-Rodrigo B., Martínez-Marín R., Delgado-Blasco J.M., Bakon M., Lazecký M., Perissin D., Papco J., Sousa J.J.: *MT-InSAR and Dam Modeling for the Comprehensive Monitoring of an Earth-Fill Dam: The Case of the Benínar Dam (Almería, Spain)*. Remote Sensing, 2023. DOI 10.3390/rs15112802. (D1, IF 5)

Infrastructure Research Lab

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- Civiš S., Lamanec Maximilián, Špirko V., Kubišta J., Špetko M., Hobza P.: *Hydrogen Bonding with Hydridic Hydrogen-Experimental Low-Temperature IR and Computational Study: Is a Revised Definition of Hydrogen Bonding Appropriate?* Journal of the American Chemical Society, 2023. DOI 10.1021/jacs.3c00802. (D1, IF 15)
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Parallel Algorithms Research Lab

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Modelling for Nanotechnologies Lab

- Hemmat M., Ayari S., Mičica M., Vergnet H., Guo S., Arfaoui M., Yu X., Vala D., Wright A., Postava K., Mangeney J., Carosella F., Jaziri S., Wang QJ., Zheng L., Tignon J., Ferreira R., Baudin E., Dhillion S.: *Layer-controlled nonlinear terahertz valleytronics in two-dimensional semimetal and semiconductor PtSe₂*. Infomat, 2023. DOI 10.1002/inf2.12468. (D1, IF 22.7)
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- Deshmukh S., Ghosh K., Pykal M., Otyepka M., Pumera M.: *Laser-Induced MXene-Functionalized Graphene Nanoarchitectonics-Based Microsupercapacitor for Health Monitoring Application*. ACS Nano, 2023. DOI 10.1021/acsnano.3c07319. (D1, IF 17.1)
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Advanced Data Analysis and Simulations Lab

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Infrastructure Research Lab

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AtoS

Advanced Data Analysis and Simulations Lab

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

Head of Lab
Number of employees

Dr Jan Martinovič
42.84 FTE

Significant activities

- Launch of the Horizon Europe project – [EXA4MIND](#), which aims to create an extreme data platform combining data storage facilities and supercomputers. The project is coordinated by IT4Innovations.
- Jan Martinovič received [an award](#) for winning the EXA4MIND project at a formal meeting of the Scientific Board of VSB-TUO.
- [Voicebot](#), also developed by researchers from IT4Innovations and activated when emergency lines are extremely overloaded, [won the award of the European DT4REGIONS initiative](#) for the most innovative solution.
- Launch of biodiversity monitoring data integration into the Digital Twin Ocean ([DTO-BioFLOW](#)) project.
- The European Space Agency (ESA) supported the [AIOPEN](#) project, on which IT4Innovations collaborates with the Space Applications Services, Telespazio, KP Labs, and SERCO companies.
- Project cooperation with the [European Space Agency \(ESA\)](#) continued under the ESA-TEP 4 Cooperation Agreement in 2023.
- The MEYS CR approved the funding of the [EOOSC-CZ](#) project, an umbrella of the international EOOSC (European Open Science Cloud) initiative in the Czech Republic. Masaryk University coordinates EOOSC-CZ.
- The Ministry of the Interior of the Czech Republic supported the [Research on Holistic Model of Interconnected Critical Electricity and Communication Infrastructures](#). The project outputs will help to understand the internal and hidden interconnections and their possible negative effects.
- The research results of the [Cell Tracking Challenge](#) initiative, which IT4Innovations is involved in, were published in the prestigious Nature Methods journal.
- In 2023, the cooperation with [Fondazione LINKS](#) (on the B-CRATOS project) continued under the Cooperation Agreement.
- [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 was developed. The research was funded by the TA CR.
- The [SmartFleet](#) platform enabling optimisation of the company's car fleet composition and full utilisation of alternative vehicles (primarily electric cars). The project was supported by the Ministry of Industry and Trade.

Infrastructure Research Lab

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

Head of Lab
Number of employees

Doc. Lubomír Říha
16.26 FTE

Significant activities

- IT4Innovations became a partner of the [MaX](#) (MAterials design at the eXascale) [Centre of Excellence](#). The centre's main activity is optimising and developing highly scalable significant community HPC applications in materials science.
- IT4Innovations became a partner of the [SPACE](#) (Scalable Parallel Astrophysical Codes for Exascale) [Centre of Excellence](#). The centre aims to prepare applications for the exascale era in astrophysics and cosmology research.
- Cooperation with ELCOM and ING corporation companies continued under the Cooperation Agreements.
- Completion of the [international SCALABLE project](#) focused on optimisation of the academic and commercial CFD software.
- [Open-source tools](#) were developed to process and visualise high-quality data and support its virtual reality (VR) presentation. Realistic visualisations (rendering) are represented by [Bheappe](#) (code.it4i.cz/raas/bheappe) and [CyclesPhi](#) (code.it4i.cz/raas/cyclesphi). The [BHolodeck](#) tool (code.it4i.cz/blender/bholodeck) allows multiple users to inspect a 3D scene in VR simultaneously.
- Collaboration with the Modelling for Nanotechnologies Lab in implementing the new Combination of Holographic and Data Safety Protection project funded by the TA CR.
- Completion of the national TA CR-funded project, in which IT4Innovations collaborated with the [IXPERTA](#) company. The project was focused on developing a software simulator for generating training data for the development of a functional sample of a detection system for railway safety.
- International cooperation in “Energy efficiency and sustainability”, focused on energy efficiency and involvement in working groups within ETP4HPC and “Power measurement methodology” within the Energy Efficiency HPC Working Group.
- Extending the monitoring of IT4Innovations' computing infrastructure and implementing [cost-saving measures reduced](#) the average consumption of the Karolina supercomputer by up to 20%.

Parallel Algorithms Research Lab

The lab 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 in combination with AI, substitution models, and digital twins in engineering applications.

Head of Lab
Number of employees

Dr Tomáš Karásek
14.78 FTE

Significant activities

- Cooperation with the [NIOB spol.s.r.o.](#) and [Model Obaly](#) companies implemented within the Cooperation Agreements.
- In 2023, the Research and development of application SW tool for efficient evaluation of catalytic processes joint project with [Orgrez a.s.](#) was completed. This project was funded by the Ministry of Industry and Trade of the Czech Republic within the Applications call.
- Newly established cooperation with the [MGL s.r.o.](#) and [FlowBox s.r.o.](#) companies in new product development in automotive and digital twins of buildings, respectively.
- The long-term cooperation with Fraunhofer ICT continued, resulting in the submission of the joint [FutureMold](#) project to the M-ERA.NET call in 2023. The project was recommended for funding and will start in mid-2024.
- Launch of the three-year [EuroCC 2](#) project, ensuring the continuation of the [National Competence Centre in HPC](#) (NCC), represented by IT4Innovations in the Czech Republic. The NCC primarily aims to offer a broad portfolio of HPC services and promote cooperation at a pan-European level, strengthening Czech companies' technological independence and competitiveness.
- The cover page of [The Journal of Physical Chemistry B](#) is adorned with a picture from the research on lipid nanoparticles by scientists from CATRIN at Palacký University Olomouc and scientists from the Modelling for Nanotechnologies Lab and the Parallel Algorithms Research Lab.
- Computational methods aimed at [solving nonlinear structural dynamical problems](#) were developed. These methods were applied to computational models of rotating machines, discretely solved using three-dimensional finite elements, to analyse their vibrations.
- An application [software tool](#) for efficient evaluation of catalytic processes was developed to provide complex support in designing SCR technologies for industrial applications. The software is based on machine learning and computational fluid dynamics (CFD) algorithms. The research was supported by the Ministry of Industry and Trade of the Czech Republic.

Modelling for Nanotechnologies Lab

The lab focuses on design, computer modelling, preparation and experimental characterisation in advanced nanomaterials and nanotechnology.

Head of Lab
Number of employees

Prof. Michal Otyepka
22.31 FTE

Significant activities

- Launch of the Experimental and theoretical studies of near-infrared emitting chiral carbon dot luminophores project under the auspices of the Moravian-Silesian Region [Global Experts](#) programme.
- The visualisation of π -holes in molecules using Kelvin probe force microscopy research, for which IT4Innovations supercomputers were also used, was published in [Nature Communications](#).
- Michal Otyepka participated in [developing a new nanomaterial](#) that instantly detects antibiotics in water.
- Scientists participated in [creating a unique technology](#) that will allow the waste from biodiesel production to be used and converted into valuable products, thus increasing the efficiency of existing biofuels. The research results were published in the Nature Communications journal.
- Within the international [s-NEBULA](#) (Horizon 2020) project, a [revolutionary approach to THz radiation detection](#) using magnetic fields was developed.
- [Novel sources of THz radiation based on spintronic effects](#), such as terahertz spintronic emitters based on spin-Hall effect and spin-laser-based THz sources, were produced and characterised.
- [New products](#), competitive in global markets, were developed [in the field of security holography](#).
- Scientists participated in developing a new [environmentally friendly method to produce hematene](#), a two-dimensional material derived from hematite, the iron mineral, with promising applications in clean energy and environmental technologies.
- A [code](#) for determining magnetostrictive and magneto-elastic coefficients in materials by quantum mechanical calculations using HPC ([MAELAS 3.0](#)) was produced.
- Dominik Legut and scientists from Charles University and the Czech Academy of Sciences contributed to a reference work on [hydride actinides](#) for the Reports on Progress in Physics journal.
- The GA CR approved the new [Novel thermoelectric, thermovoltaic, and phonoelectric heat conversion systems based on nitride semiconductors](#) project for funding. The TA CR supported the [Combination of Holographic and Data Safety Protection](#) project. MIT CR approved the [Terahertz Raman spectrometers with enhanced application capabilities](#) project for funding.

Big Data Analysis Lab

The lab was focused on network security, the Internet of Things, big data analysis, speech processing, and artificial intelligence applications in complex systems. It also aimed at developing efficient knowledge acquisition and processing methods.

At its meeting on 19 December 2023, the Academic Senate of VSB – Technical University of Ostrava approved transforming the Big Data Analysis Lab into the Quantum Computing Lab.

Head of Lab
Number of employees

Prof. Miroslav Vozňák
2.98 FTE

Significant activities

- Completion of the Horizon 2020 [OpenQKD](#) (Open European Quantum Key Distribution Testbed) project. The project has created a testbed for a highly secure network using quantum mechanical principles for key distribution. The HPC use case via QKD between IT4Innovations and PSNC (Poznan) was implemented. Furthermore, IT4Innovations collaborated on the development and implementation of key management. The third domain was the simulation of implemented QKD deployment cases for all partners in the project, as well as the enhancement of the QKD simulator, which is being developed as an open source in Ostrava. IT4Innovations computational resources were used in the simulations. As part of the project, another version of the QKD network simulator ([open-qkd.eu](#)) was released in 2023. This simulator allows the decomposition of QKD network components into layers (QKD link, KMS link, and QKD user).
- Completion of the [Artificial Intelligence and Reasoning](#) project, supported by the MEYS of the Czech Republic, which dealt 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.
- Miroslav Vozňák, as an invited keynote speaker, presented the Population Mobility Retrieval from Mobile Network paper at the ICUMT symposium in Ghent, Belgium. He was also an invited speaker at the PTV Rail Summit, which discussed the use of processed population mobility data for high-speed line planning.



↔ The REFRESH project

The REFRESH project, led by VSB-TUO, has received funding of CZK 2.5 billion from the Just Transition Operational Programme and is the largest project in the history of VSB-TUO. The project aims to respond to the region's problems and contribute to its successful economic, energy, and environmental transformation. The project is based on four interconnected living labs where cutting-edge research is carried out in close contact with companies and in accordance with the requirements of end users. IT4Innovations and the Centre for Energy and Environmental Technologies lead the Energy Lab's Digitalisation and Energy Transformation research programme.

6

Educational and Training Activities

IT4Innovations has long been involved in various educational and training activities. Our experts teach VSB – Technical University of Ostrava students within MSc and PhD study programmes. In 2023, we organised **33 trainings, seminars, and workshops dedicated to HPC, HPDA, QC, and AI** as part of professional education. Another seven events were held within the EOOSC-CZ Training Centre, where IT4Innovations coordinates the education of a broad scientific community in the Czech Republic on specialised topics in the area of open science and FAIR data.

Educational activities

IT4Innovations and the Faculty of Electrical Engineering and Computer Science at VSB-TUO prepared and successfully accredited the **Informatics and Computational Sciences** PhD study programme, which focuses on using HPC, HPDA, and AI in science and industry. In 2023, 7 students studied in the ongoing **Computational Sciences** PhD study programme, with 2 completing their studies.

Experts from IT4Innovations are involved in teaching students within the **Computational and Applied Mathematics** MSc study programme. The Department of Applied

Mathematics at the Faculty of Electrical Engineering and Computer Science at VSB-TUO guarantees the programme. In 2022, the new **Introduction to Quantum Computing** course was prepared. In 2023, the first students from the Faculty of Electrical Engineering and Computer Science at VSB-TUO enrolled in the course.

IT4Innovations is a member of an international consortium implementing the 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. Starting from the 2022 winter semester, the MSc study programmes are provided by eight European universities. In 2023, another cohort of students began their studies, and at the end of 2023, it was decided that the third batch of students would start their studies in the autumn of 2024. Participation of the Czech Republic in the European EuroHPC Joint Undertaking enables Czech students to enrol in this study programme. Graduates will find careers in fast-growing fields such as HPC, HPDA, and AI. This project is part of a more comprehensive EuroHPC JU strategy facilitating the development of critical 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 EuroCC2, 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 newly also in quantum computing.

In 2023, IT4Innovations held **33 educational events and workshops** attended by **873 participants**, whether in person or online. Compared to the last year, the number of events offered is almost a two-fold increase. A total of 23 educational events were held under the auspices of the National Competence Centre in HPC (EuroCC2 project), five events under the auspices of the IO-SEA project, three events within the European Digital Innovation Hub Ostrava (EDIH Ostrava), one event thanks to the SCtrain project, and one under the UrbanTEP project.

Division of training by area

16 HPC 7 AI 7 QC 3 HPDA

In 2023, IT4Innovations renewed cooperation with partners from Slovakia and Poland in the **Superheroes 4 Science** project. This time, the partners will focus on developing fun, interactive educational materials for primary and secondary school teachers to help teach the basic principles of quantum computing and artificial intelligence. We are also educating future generations of scientists by hosting **Introduction to Quantum Computing** workshops, which last year were attended by nearly 100 high school students.

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 (2023–2026)

→ Project ID: LM2023054
→ Principal Investigator: Doc. Vít Vondrák

→ e-INFRA CZ is a unique e-infrastructure for research, development, and innovation in the Czech Republic. It creates a communication, information, storage, and computing platform for research, development, and innovation both nationally in the Czech Republic and internationally and provides an extensive and comprehensive portfolio of ICT services without which modern research, development, and innovation cannot be conducted. The main components of e-INFRA CZ include: a high-performance national communication infrastructure, a national grid and cloud infrastructure, the most powerful and advanced supercomputing systems in the Czech Republic, and high-capacity data storage.

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's objective was to modernise and develop the capacity of all e-infrastructure components so that the level of IT infrastructure support corresponds to the predicted requirements of the user community for the given period and simultaneously to the state-of-the-art level of the field.

e-INFRA CZ II Modernisation (2023–2026)

Projects of the Operational Programme Johannes Amos Comenius

→ Project ID: CZ.02.01.01/00/23_016/0008329
→ Principal Investigator: Doc. Vít Vondrák

→ The project aims to modernise and upgrade the e-INFRA CZ e-infrastructure, a strategic infrastructure for research, development, and innovation in the Czech Republic. It will modernise specific components, such as supercomputers and their facilities.

Research and Development Projects

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

Projects of the Operational Programme Johannes Amos Comenius

European Open Science Cloud Czech Republic (2023–2028)

→ Project ID: CZ.02.01.01/00/22_004/0007682
→ Principal Investigator: Dr Kateřina Slaninová

European Open Science Cloud (EOSC) is a European initiative focused on developing infrastructures supporting open science practices in research data management. It offers facilities for storing and sharing FAIR research data – findable, accessible, interoperable, and reusable. The EOSC-CZ project is the implementation of the EOSC initiative in the Czech Republic, which aims to create a national node of this European initiative and promote good practice in research data management across scientific communities. Within Implementing National Data Infrastructures (NDI), a common platform for sharing, managing, and accessing data and computational resources for research purposes will be created. The NDI will support scientific and multidisciplinary research activities and include various scientific fields and disciplines.

→ www.eosc.cz

Projects of the Operational Programme Research, Development, and Education

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 Artificial Intelligence and Reasoning research within a given part of the Czech Institute of Informatics, Robotics, and Cybernetics (CIIRC), solving advanced interdisciplinary problems of high technical and 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 stemmed from the emphasis on the concentration and integration of resources, sharing of knowledge, and infrastructure and establishing a “unified space for opportunities” for young talents in the Czech Republic.

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 Faltýnková

→ The project aimed to create open-source tools that would allow data to be processed and visualised in high quality and support its presentation in virtual reality (VR). The developed tools were explicitly focused on medical data visualisation, HPC cluster runtime monitoring, and visualisation of simulation results from parallel open-source simulation tools. The primary objective of the project included high-quality visualisations in VR. Within the project, resource consumption monitoring of IT4Innovations supercomputers and their visualisations were also activated. This feature, which is greatly appreciated by both administrators and users of these systems, allows 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

→ Within the project, THz sources using spintronic phenomena, such as terahertz spintronic emitters based on the spin-Hall effect and spin laser-based THz sources, were designed, developed, and characterised. Photonic and plasmonic structures were used to enhance the performance of these devices, including Bragg grating and plasmonic materials for spintronic emitters and anisotropic 2D gratings for spin lasers. Non-conventional characterisation methods were used to describe the spin momentum and broadband optical properties, including terahertz plasma-based time-domain spectroscopy and the resulting pump-probe measurements.

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 project aimed to develop computational procedures to solve non-linear structural, dynamical problems, which were subsequently applied to computational models of rotating machines discretised by three-dimensional finite elements to analyse their vibrations. The methods were developed and studied on test cases in the MATLAB software and subsequently implemented in ESPRESO (ExaScale PaRallel FETI SOLver) developed as an open-source code at IT4Innovations and tested on real industrial cases.

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

→ The project aims to explore and explain the role of 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.



[↔ Visit](#)

IT4Innovations hosted a debate with Ivan Bartoš, Deputy Prime Minister of the Czech Republic for Digitalisation, in the framework of the Week for Digital Czechia.

Experimental and theoretical studies of near-infrared emitting chiral carbon dot luminescence project (2023–2026)

Projects supported by the Moravian-Silesian Region
Global Experts Programme

→ Project ID: 00734/2023/RRC
→ Principal Investigator: Prof. Michal Otyepka

→ The project brings together the expertise of carbon dot synthesis specialists, who will focus on preparing dots with high quantum emission yields, particularly in the red and near-infrared, and on chiral carbon dots for sensing applications. These efforts will be supported by state-of-the-art materials characterisation techniques to determine carbon dots' composition, structural properties, and electronic and ultrafast optical properties. This will be done in close collaboration with a theoretical computing group with expertise in complex structural models of a wide range of photoluminescent materials. This project serves as a means of transferring the know-how and bringing the expertise of Professor Andrey Rogach's group to VSB-TUO by importing their skills in materials and their characterisation and by creating a close collaboration between the teams involved.

Projects supported by the Grant Agency of the Czech Republic
International grant projects evaluated by the LEAD Agency principle

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

→ The project aims to study and develop a quantitative theory of coercivity regarding the local atomic structure (grain boundary, grain size) and its influence on the spatial variation of the intrinsic magnetic properties and microstructure. 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: 22-22322S
→ Principal Investigator: Dr Dominik Legut

→ 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_2 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.

Magnetism at Interfaces: from quantum to reality (2022–2025)

Unconventional superconductors under extreme conditions (2022–2024)

Novel thermoelectric, thermovoltaic, and photoelectric heat conversion systems based on nitrides semiconductors (2023–2025)

→ Project ID: 23-07228S
→ Principal Investigator: Dr Dominik Legut

→ This project focuses on developing n-type and p-type semiconductors based on doped ScN and CrN for heat transfer applications. Theoretical research based on state-of-the-art quantum mechanical density functional theory calculations will be performed to support and complement the experimental part. Finally, the first development of p-n junctions for heat transfer will be carried out using the results obtained on the tested materials.

Projects supported by the Technology Agency of the Czech Republic
TREND Programme

→ Project ID: FW06010089
→ Principal Investigator: Doc. Kamil Postava

→ The project will increase the use of modern digital technologies in the product offer of Optaglio a.s., thus increasing its competitiveness, especially in foreign markets. The aim is to prevent the possibility of counterfeiting of holographic security features by their individual connection with the digital database. This linking requires the development of new ways of writing a completely random and non-repeatable motif, its conversion into digital form using the image hashing function, fast reading of the motif, preferably using a standard mobile phone, and subsequent writing and comparison with the digital (de)centralised database.

ÉTA Programme

→ Project ID: TL05000184
→ Principal Investigator: Prof. Marek Lampart

Combination of Holographic and Digital Safety Protection (2023–2025)

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)

→ The project aimed to create a comprehensive research report and software for the needs of the Ministry of Labour and Social Affairs in implementing family policy 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 serve as essential material for creating a model of the tax-benefit system implemented in software, of which the primary purpose is 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.

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

SmartFleet – AI-based software for 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 objective was to create a SmartFleet platform enabling 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 was 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 – from purchase planning and daily planning to online monitoring and reaction to all daily changes.

Holograms with active safety elements (2021–2023)

→ Project ID: CZ.01.1.02/0.0/0.0/20_321/0024953
→ Principal Investigator: Doc. Kamil Postava

→ The aim of the joint industrial research project of Optaglio a.s. and VSB-TUO was to develop new products in the field of security holography that would be competitive on global markets. These are entirely new types of anti-counterfeiting features. The project was focused 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 effective 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 aimed to create a SW tool for the effective evaluation of catalytic processes and for comprehensive support in designing SCR technologies for industrial applications. The research and development activities solved the overall DeNOx process by reducing nitrogen oxides from the exhaust gases when reacting with gaseous NH₃. The SW uses machine learning algorithms and flow calculations (CFD). The SW has a direct commercial application in nitrogen emission reduction solutions in power plants in the Czech Republic and abroad.

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 aimed to conduct research and development activities in cloud and printing solutions. It was implemented in effective collaboration with Y Soft Print Management Solutions, a.s., VSB-TUO, and Czech Technical University in Prague.

Terahertz Raman spectrometers with enhanced application capabilities (2023–2025)

Projects of the Operational Programme Technologies and Application for Competitiveness

→ Project ID: CZ.01.01.01/01/2_2_002/0000605
→ Principal Investigator: Doc. Kamil Postava

→ The project is a continuation of a successful, more than 10-year cooperation between the ZEBR s.r.o. company, Palacký University, and VSB-TUO in developing an instrument for spectral analysis of substances using Raman optical activity (ROA) detection.

Projects supported by the Ministry of the Interior of the Czech Republic

→ Project ID: VK01030109
→ Principal Investigator: Dr Pavel Praks

→ The project brings together three research centres (CVOOZE, SIX, and IT4I) and creates an interdisciplinary research team with available know-how (in modelling, energy, communications, and high-performance computing) focused on exploring the interconnectedness of individual critical infrastructures (control, data, and energy) to enhance resilience, robustness, and preparedness against potential risks, threats, and domino effects. The project outputs will help us understand the internal and hidden interdependencies and their possible negative effects. The results will be used in planning, optimising, and extending these critical infrastructures through the user organisations involved, from both the public and private sectors. The socio-scientific contribution of the project is guaranteed by the openness of the solutions considered concerning the principles of open science.

VSB-TUO Projects with IT4Innovations Participation

Energy System for Grids (2019–2023)

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

→ The project aimed 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 supports 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 energy sources. The project's objective was to ensure 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.

REFRESH – Research Excellence For Region Sustainability and High-tech Industries (2022–2027)

- Project ID: CZ.10.03.01/00/22_003/0000048
- IT4I Coordinator: Prof. Tomáš Kozubek
- Grant Provider: Ministry of the Environment (State Environmental Fund of the Czech Republic), Operational Programme Just Transition 2021–2027

→ The REFRESH project is a key tool for implementing the SMARAGD strategy, which contributes to transforming the Moravian-Silesian Region (MSR) into a SMART And Green District. The main objective of the REFRESH project is to create a robust innovation ecosystem in the MSR in four domains of specialisation: new energy, automation and robotics in manufacturing and transport, digitalisation, novel materials, and environmental technologies, including their socio-economic dimension. These domains are part of the MSR's smart specialisation strategy. An integral part of the REFRESH project and its uniqueness is the emphasis on the integration of the social dimension into all activities. The individual and societal capacity to adapt to conditions of dynamic technological development will significantly influence the project's overall contribution to the region's transformation.

Validation of integrating artificial intelligence for receiving emergency calls using a voice chatbot, developed within the research project BV No. VI20192022169, with technology for receiving emergency communications 112 and 150 in the Czech Republic (TCTV 112) (2023–2025)

- Project ID: VK01020132
- Principal Investigator: Petr Berglowiec (Faculty of Safety Engineering, VSB-TUO)
- Grant Provider: Ministry of the Interior of the Czech Republic

→ The project deals with artificial intelligence for receiving emergency calls. It follows up the results of Research Project No. VI20192022169, and its objective is to integrate voice chatbot into the technologies for lines 112 and 150 in the Czech Republic (TCTV 112) with a focus on the use of geolocation to refine speech recognition and dialogue, collaborative chatbot supported by human operators in named-entity recognition, detection of topics enabling the transfer of a call to a human operator for issues outside of the chatbot's competence, and language identification. The project will also examine the interaction of human and automated operators in scenarios of verification and human supervision of one or more voice bots. The project is primarily dedicated to voice communication but will also deal with emergency SMS. Its outputs include two software demonstrators.

International Projects

Supercomputing Services Projects

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

- Project ID: 101017207 (H2020-INFRAEOSC-2018-2020, RIA)
- Principal Investigator: Filip Staněk

→ The project consortium brought together a network of computing and data centres, research infrastructures, and data repositories to enable a European storage and data management infrastructure for EOSC in data management and storage, providing generic services and building blocks to store, find, access, and process data consistently and persistently.

→ www.dice-eosc.eu

Research and Development Projects

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

- 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 maintain Europe's worldwide leadership in Computer-Aided Drug Design (CADD) solutions exploiting today's high-end supercomputers and tomorrow's exascale supercomputers, thus fostering European competitiveness in this field. The proposed LIGATE fully integrated solution enables the delivery of the drug design campaign results with the highest speed and accuracy and autotuning of the solutions' parameters to meet the time and resource constraints.

→ www.ligateproject.eu

LIGATE – Ligand Generator and portable drug discovery platform AT Exascale (2021–2024)

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 a high-tech and especially secure system for High-Performance Data Analysis. This will be achieved by simplifying the programmability of heterogeneous and distributed architectures through a data-driven design approach, using hardware-accelerated artificial intelligence, and efficiently monitoring execution with a unified hardware-software paradigm. The project will validate its approach through three case studies: a weather-based prediction model, an air quality monitoring application, and a traffic modelling framework for smart cities.

→ www.everest-h2020.eu



↔ 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 can access one of the world's most powerful and advanced supercomputers; the theoretical peak performance reached 531.5 PFlop/s in 2023.

**ACROSS – HPC big data
artificial intelligence cross stack
platform toward
exascale (2021–2024)**

- Project ID: 955648 (H2020-JTI-EuroHPC-2019-1, EuroHPC-IA)
- Principal Investigator: Dr Jan Martinovič

→ The project proposes and develops a High-Performance Computing (HPC), Big Data (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 supercomputers, 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

**s-NEBULA – Novel
Spin-Based Building
Blocks for Advanced
TeraHertz Applications (2020–2023)**

- Project ID: 863155 (H2020-FETOPEN-2018-2020, RIA)
- Principal Investigator: Doc. Kamil Postava

→ The project aimed to research and develop a revolutionary approach to spin-based TeraHertz (THz) technology for generating and detecting THz radiation. The project plan was to create a platform for room-temperature innovative spin-based THz building blocks arising from novel combinations of magnetism and optics. The project aimed to provide cutting-edge solutions to solve bottleneck scientific issues in THz technologies motivated by explicit needs in judiciously chosen target applications. → 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 brought together renowned industrial and academic partners to improve the performance, scalability, and energy efficiency of industrial Lattice Boltzmann method-based computational fluid dynamics (CFD) software. The Lattice Boltzmann method (LBM) provides a reliable alternative to conventional CFD approaches. The LBM is generally well-suited to exploit advanced supercomputer architectures as it enables massive parallelisation. The project directly benefited European industry and contributed to fundamental research.

→ www.scalable-hpc.eu

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

- Project ID: 955811 (H2020-JTI-EuroHPC-2019-1, EuroHPC-RIA)
- Principal Investigator: Dr Jan Martinovič

→ The project aims to provide a novel data management and storage platform for exascale computing based on hierarchical storage management and on-demand provisioning of storage services. The platform will efficiently use storage tiers spanning NVMe and NVRAM at the top and tape-based technologies all the way down. 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

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

→ Project ID: 857156 (H2020-SU-ICT-2018-2020)
→ Principal Investigator: Prof. Miroslav Vozňák

→ The project aimed 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. The role of IT4Innovations was primarily in three areas. The first was a real use case of HPC via QKD between IT4Innovations and PSNC (Poznan, Poland). The second was the participation in developing and implementing key management. The third domain was a simulation of the QKD use cases of all project partners and the improvement of an open-source QKD simulator being developed in Ostrava. The computational resources of IT4Innovations were used for the simulations. → www.openqkd.eu

EUPEX – European Pilot for EXascale (2022–2026)

→ Project ID: 101033975 (H2020-JTI-EuroHPC-2020-01, RIA)
→ Principal Investigator: Doc. Lubomír Říha

→ The project consortium aims to design, build, and validate the first EU platform for High-Performance Computing (HPC), covering end-to-end the spectrum of required technologies with European assets, from the architecture, processor, system software, and development tools to 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

Projects of the 9th 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

→ The project aims to push the current boundaries of a predictive understanding of biodiversity dynamics by developing a Digital Twin that will provide advanced modelling, simulation, and prediction capabilities. By exploiting existing technologies and data available across relevant research infrastructures in new ways, the project will enable the interaction between species and their environment to be modelled accurately. Thus, scientists will use BioDT to observe biodiversity changes better, relate these changes to possible causes, and better predict the effects of these 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. → 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 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 search engine-based application market. Within three years, the researchers will develop the core of the European Open Web Index as a basis for a new Internet Search in Europe. In addition, the project will lay the foundation for an open and extensible European Open Web Search and Analysis Infrastructure based on Europe’s values, principles, legislation, and standards. → openwebsearch.eu

EXA4MIND – Extreme Analytics for MINING Data spaces (2023–2025)

→ Project ID: 101092944 (HORIZON-CL4-2022-DATA-01, RIA)
→ Principal Investigator: Dr Jan Martinovič

→ The project will build an Extreme Data platform connecting data storage facilities and supercomputers by introducing new methods for automated data management and effective data staging. The project’s core consists of four application cases in molecular dynamics, advanced driver assistance systems, smart agriculture/viticulture, and health and social big data. The project presents innovative solutions to complex everyday data-processing problems using advanced data analytics, machine learning, and artificial intelligence to simplify using supercomputing centres in the EU for applications dealing with extreme data. → www.exa4mind.eu

SPACE – Scalable Parallel and distributed Astrophysical Codes for Exascale (2023–2026)

→ Project ID: 101093441 (HORIZON-EUROHPC-JU-2021-COE-01)
→ Principal Investigator: Doc. Lubomír Říha

→ In astrophysics and cosmology, High-Performance Computing-based numerical simulations are key tools for scientific discovery. They represent essential tools for theoretical experiments capable of understanding physical processes behind the observed sky, for which the effective exploitation of exascale computing capabilities is necessary. These systems, however, have a complicated architecture that significantly impacts simulation codes. The SPACE Centre of Excellence aims to re-engineer target codes to fully utilise new computer architectures and apply new programming methods, software solutions, and HPC libraries. → www.space-coe.eu

MaX – MAterials design at the eXascale (2023–2026)

→ Project ID: 101093374 (HORIZON-EUROHPC-JU-2021-COE-01)
→ Principal Investigator: Doc. Lubomír Říha

→ Materials simulations have become one of the most intensive and fast-growing domains for high-performance computing worldwide, with a recognised European leadership in developing and innovating the ecosystem of quantum simulation codes. The MaX project will target these flagship codes to address the challenges, leverage the opportunities arising from future exascale and post-exascale architectures, and offer powerful paths to discovery and innovation serving scientific and industrial applications. → www.max-centre.eu

DTO-BioFlow – Integration of biodiversity monitoring data into the Digital Twin Ocean (2023–2027)

→ Project ID: 101112823 (HORIZON-MISS-2022-OCEAN-01, IA)

→ Principal Investigator: Dr Tomáš Martinovič

→ The project's primary objective is to awaken sleeping biodiversity data, enabling a smooth integration of both existing and new data into the European Digital Twin Ocean. The project will provide innovative and sustainable solutions for making previously unavailable or hard-to-access biodiversity data accessible. Additionally, it will focus on developing cost-effective and scalable technologies for monitoring species on a large scale. The project aims to improve the European biodiversity data environment by streamlining the flow of FAIR data from various sources into digital twin repositories, optimising and enhancing the functionality and societal value of the Digital Twin Ocean. → dto-bioflow.eu

Digital Europe Programme

EUROCC2 – National Competence Centres in the Framework of EuroHPC Phase 2 (2023–2025)

→ Project ID: 101101903 (DIGITAL-EUROHPC-JU-2022-NCC-01)

→ Principal Investigator: Dr Tomáš Karásek

The mission of EuroCC 2 is to continue establishing a network of National Competence Centres in the most efficient way possible while continuing to promote an efficient way to spread High-Performance Computing (HPC) in Europe. The main objective is to leverage the experience and expertise in the HPC field, which is a stepping stone for the primary purpose: to support the National Competence Centres in developing their individual operational frameworks, to develop further cooperation and exchange of good practice, and to accelerate the process of competence development at national and European level. → www.eurocc-access.eu

CZQCI – Czech National Quantum Communication Infrastructure (2023–2026)

→ Project ID: 101091684 (DIGITAL-2021-QCI-01, DIGITAL Simple Grants)

→ Principal Investigator: Doc. Vít Vondrák

→ The project will enable the introduction of quantum communication infrastructure (QCI) in the Czech Republic. A training programme will be designed and developed to prepare users and professionals from all sectors to use future quantum communication infrastructures. The infrastructure and expertise gained through the project will allow for testing advanced communication methods between public authorities and industrial users, testing operational requirements in terms of long distances and time, and testing QKD and network components. The highly demanding pilot testing will pave the way for the widespread deployment of QCI. The project will significantly increase cyber security in Europe by promoting and deploying European quantum communication technologies.

EDIH Ostrava – European Digital Innovation Hub Ostrava (2023–2025)

→ Project ID: 101083551 (DIGITAL-2021-EDIH-01)

→ Principal Investigator: Martin Duda

→ The mission of the European Digital Innovation Hub Ostrava (EDIH Ostrava) is to support the deployment and use of advanced digital technologies in companies and society. The EDIH Ostrava offers its services under highly favourable subsidised conditions or free of charge. It was created by combining the activities of IT4Innovations, the Faculty of Electrical Engineering and Computer Science, which are part of VSB-TUO, and the Moravian-Silesian Innovation Centre Ostrava. → www.edihostrava.cz

SCtrain – Supercomputing knowledge partnership (2020–2023)

Educational Projects

Erasmus+ Projects

→ Project ID: 20-203-075975 (KA203-6E6A1FFC)

→ Principal Investigator: Prof. Tomáš Kozubek

→ The mission of this project was to use a methodical approach to fill gaps in current university courses and increase awareness of HPC for future professionals in science and technology.

→ sctrain.eu

Projects of the 8th Framework Programme for Research and Innovation 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 of universities, research and supercomputing centres, industrial partners, and other cooperating institutions aims to launch master's study programmes at eight European universities. This activity is part of the broader EuroHPC JU strategy, which supports the development of critical competencies and education and training in HPC to meet the needs of European science and industry.

→ eumaster4hpc.uni.lu

International Visegrad Fund

Superheroes 4 Science (2023–2025)

→ Project ID: 22320170 (International Visegrad Fund)

→ Principal Investigator: Karina Pešatová, MBA

→ The project aims to introduce the young generation to High-Performance Computing (HPC), a critical technology field that uses supercomputers to solve complex problems and perform computationally intensive tasks. It also aims to create interactive educational materials on HPC and its two related emerging fields: Artificial Intelligence and Quantum Computing. → superheroes4science.eu

List of Abbreviations

AI	Artificial Intelligence
AIOOPEN	European Space Agency project
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
CATRIN	Czech Advanced Technology and Research Institute
CEET	Centre for Energy and Environmental Technologies
DICE	Data Infrastructure Capacity for EOSC
DOI	Digital Object Identifier
DTO-BioFLOW	Integration of biodiversity monitoring data into the Digital Twin Ocean
DT4REGIONS	European initiative supporting the use of AI in public administration
EDIH Ostrava	European Digital Innovation Hub Ostrava
e-INFRA CZ	e-infrastructure for research and development in the Czech Republic
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	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
Flop/s	Floating-point operations per second
FP7	Seventh Framework Programme for Research and Technological Development
FTE	Full-Time Equivalent
GA CR	Grant Agency of the Czech Republic (Czech Science Foundation)
GPU	Graphics Processing Unit
H2020	Horizon 2020
HPC	High-Performance Computing
HPDA	High-Performance Data Analytics
ICT	Information and communication technology
IF	Impact Factor, an indicator that reflects the quality of scientific publications
IO-SEA	IO Software for Exascale Architecture
iRODS	Integrated Rule-Oriented Data System
LEXIS	Large-scale EXecution for Industry & Society
LIGATE	Ligand Generator and portable drug discovery platform AT Exascale
LUMI	Large Unified Modern Infrastructure
LUMI-C	LUMI partition using only CPU-based compute nodes
LUMI-G	GPU-accelerated LUMI partition
LUMI-Q	Large Unified Modern Infrastructure for Quantum Computing
MaX	MAterials design at the eXascale, European Centre of Excellence
MEYS	Ministry of Education, Youth and Sports of the Czech Republic
MI CR	Ministry of Interior of the Czech Republic

MIT	Ministry of Industry and Trade of the Czech Republic
MPI	Message Passing Interface, programming model
MSR	Moravian-Silesian Region
OPENQKD	Open European Quantum Key Distribution Testbed
POP3	Performance Optimisation and Productivity 3, European Centre of Excellence
PRACE	Partnership for Advanced Computing in Europe
PRACE-6IP	Partnership for Advanced Computing in Europe, 6 th Implementation Phase
QKD	Quantum Key Distribution
SCALABLE	SCALable LAttice Boltzmann Leaps to Exascale
SCtrain	Supercomputing Knowledge Partnership
s-NEBULA	Novel Spin-Based Building Blocks for Advanced TeraHertz Applications
SPACE	Scalable Parallel Astrophysical Codes for Exascale, European Centre of Excellence
SW	Software
SWP	Sequential Write Performance
SRP	Sequential Read Performance
TA CR	Technology Agency of the Czech Republic
THz radiation	Terahertz radiation
R&D	Research and Development
R&D&I	Research, development, and innovation
VR	Virtual reality
VSU-TUO	VSU – Technical University of Ostrava



www.it4i.eu

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MINISTRY OF EDUCATION,
YOUTH AND SPORTS