Review 2024

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

Empowering innovations with the Karolina and Barbora supercomputers and the VLQ quantum computer

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IT4I

MANAGING DIRECTOR'S INTRODUCTION

Dear colleagues, partners, and friends,

It is my pleasure to present to you an overview of the activities of IT4Innovations National Supercomputing Center for the year 2024. A year marked by several milestones, expansion of our research efforts, and deeper involvement in more intensive collaboration on the European stage in the development and application of supercomputing technologies. Once again, we demonstrated that our expertise in high-performance computing, artificial intelligence, data analysis, and quantum computing holds a firm place in Europe. It also confirmed our success in fulfilling our mission: to provide state-of-the-art computing infrastructure and expertise not only for the Czech but also for the European research and innovation community.

Among the most significant milestones was the progress in quantum technologies. In September, the EuroHPC Joint Undertaking (EuroHPC JU) signed a contract with the IQM Quantum Computers company for the delivery of the VLQ quantum computer of the LUMI-Q consortium, which will be installed and operated directly at our centre. This represents not only a technological but also a strategic breakthrough, positioning us as a key European node in quantum computing. At the same time, we deployed the NVIDIA CUDA Quantum simulator on the Karolina supercomputer, establishing an environment for the development of hybrid applications and increasing the productivity and scalability of quantum computations.

The year 2024 also marked the beginning of our participation in creating the EuroHPC Federation Platform, which we are developing together with other partners for the EuroHPC JU. The aim is to build and operate a unified environment for accessing all EuroHPC computational resources including integration into European data infrastructures.

Another important development is our involvement in the emerging European CLARA Centre of Excellence, which focuses on research into neurodegenerative diseases using the latest tools in artificial intelligence and quantum computing. As part of this project, we are building the so-called CLARA Testbed. In addition to acquiring a new computing cluster and data storage system for our centre, it will also connect the computational and data resources of project partners and other research communities focused on related topics.

In 2024, we also contributed to more than twenty international research projects. We launched the FALCON project aimed at enhancing the competitiveness of the European aerospace industry, the EPICURE project focused on supporting EuroHPC JU supercomputer users through collaboration and shared expertise, and the AVITHRAPID project, which seeks to accelerate the discovery of antiviral compounds using supercomputing technologies.

The outcomes of our work were presented in leading scientific journals and even featured on the covers of ChemPhysChem and the Journal of the American Chemical Society. In the field of numerical simulations, we developed an innovative method to optimise the performance of the finite element method, achieving up to an eightfold increase in speed. We also joined the VI-HPS initiative to improve productivity in supercomputing applications through our long-term development of the MERIC software package. Within the LIGATE project, we demonstrated breakthrough LIGEN computations running in parallel on the LUMI, Karolina, Leonardo, and E4 supercomputers. In cooperation with partners, we also launched a new web server, AggreProt, designed to predict protein aggregation.

We also honour our commitment to the region. Along with other departments of VSB-TUO, we participated in implementing the REFRESH project focused on transforming the Moravian-Silesian Region. Cooperation with industry remains one of our pillars. In 2024, through the European Digital Innovation Hub Ostrava and the National Competence Centre in HPC, we supported companies and start-ups across various sectors, from healthcare and energy to the automotive industry. We help companies harness the power of supercomputers and accelerate innovation in practice.

We also devoted considerable attention to education and public engagement. We organised the HPC in Data Science summer school within the EUMaster4HPC project, welcomed several hundred visitors during the Researchers' Night, and organised the sixth annual HPCSE scientific conference. We also contributed actively to the development of the sixth edition of the European Strategic Research Agenda within ETP4HPC, which outlines the current European ecosystem for high-performance computing, artificial intelligence, and quantum computing. Furthermore, we helped establish the Central European chapter of the Women in High Performance Computing network, which I consider a key step toward supporting diversity and equality in our field.

Finally, allow me to express my sincere gratitude to all our colleagues, partners, and supporters. Thanks to you, we can continue to build IT4Innovations as a centre of excellence and innovation. We look forward to another year of collaboration, growth, and scientific discovery.

Sincerely,

Vít Vondrák

Managing Director

The IT4Innovations building

01

IT4INNOVATIONS PROFILE

IT4Innovations

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 in the field of High-Performance Computing (HPC), High-Performance Data Analysis (HPDA), Quantum Computing (QC), and Artificial Intelligence (AI), including their applications in science, industry, and society. Since 2013, IT4Innovations has been providing state-of-the-art supercomputing technologies and services both Czech and international research teams from academia and the private sector, with the goal of boosting competitiveness and fostering innovation in 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 currently operates two supercomputers, which are scheduled for modernisation in 2025 and 2026. The **Karolina** supercomputer, installed in summer 2021, achieves a theoretical computing performance of 15.7 PFlop/s, while **Barbora**, launched in autumn 2019, offers 849 TFlop/s. As a member of the LUMI consortium, IT4Innovations also participates in operating **LUMI**, one of Europe's most powerful supercomputers, located in Kajaani, Finland. Thanks to this, the Czech research community has access to this system, which offers a peak performance of 531.5 PFlop/s.

Within its data room, IT4Innovations also operates **complementary systems** composed of several different hardware platforms. These complementary systems provide users with access to emerging, non-traditional, and highly specialised hardware architectures.

The first quantum computer in the Czech Republic, named VLQ, is being installed at IT4Innovations in 2025. VLQ is part of the LUMI-Q consortium, which comprises 13 partners from eight European countries. The **VLQ quantum computer** is based on 24 superconducting qubits in a star-shaped topology. Its integration with the Karolina supercomputer is also planned, as well as potential integration with other supercomputers within and beyond the LUMI-Q consortium.

IT4Innovations is also one of the partners of the **LUMI AI Factory**, representing an innovative infrastructure and support centre aimed at accelerating the adoption of AI tools across Europe. It enables startups, SMEs, researchers, and companies to develop advanced AI models, tools, and applications. IT4Innovations is one of the active partners involved in the establishment and operation of the LUMI AI Factory.

IT4Innovations has been involved in preparing the **EuroHPC Federation Platform** for the EuroHPC JU. This assignment is aimed at federating all EuroHPC supercomputing and quantum systems, including AI Factories, and their connection to European data infrastructures. The objective is to unify and simplify access to all computing and data resources operated by the EuroHPC JU.

The core research topics at IT4Innovations include large-scale data processing and analysis, machine learning, and AI, the development of scalable parallel algorithms and algorithms for quantum computers and simulators, solving challenging engineering tasks, advanced visualisation and virtual reality, the development of new materials, and energy efficiency of supercomputing technologies.

In 2024, research activities at IT4Innovations were carried out in five research laboratories:

IT4Innovations is a member of the MaX, SPACE, POP3, and CLARA Centres of Excellence. Within the CLARA Centre of Excellence, a Testbed is being established at IT4Innovations, which will serve the scientific community researching neurodegenerative diseases through quantum and classical supercomputing. Additionally, IT4Innovations is a partner in over **20 international projects** under Horizon 2020, Horizon Europe, and Digital Europe programmes, coordinating projects such as EXA4MIND and EDIH Ostrava.

IT4Innovations actively cooperates with industry. Experts from the **European Digital Innovation Hub Ostrava** (EDIH Ostrava) and the **National Competence Centre in HPC** are available to assist, especially SMEs and startups, by providing a wide range of services in supercomputing and in the adoption and application of digital technologies.

IT4Innovations has long organised and offered a wide array of specialised training events focused on HPC, HPDA, AI, and QC, and on acquiring skills necessary for the effective use of supercomputing infrastructure. It also focuses on developing digital skills. In these areas, IT4Innovations is actively involved in educating students, particularly through study programmes at VSB – Technical University of Ostrava. IT4Innovations is also a member of the EUMaster4HPC consortium, which implements the eponymous pan-European MSc study programme focused on high-performance computing.

RESEARCH LABS:

- Advanced Data Analysis and Simulations Lab
- Infrastructure Research Lab
- Parallel Algorithms Research Lab
- Modelling for Nanotechnologies Lab
- Quantum Computing Lab

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 Joint Undertaking (EuroHPC JU), with IT4Innovations playing a significant role in its activities
- IT4Innovations becomes part of the H2020 POP2 Centre of Excellence

2019
- Launch of the Barbora supercomputer and the NVIDIA DGX-2 system
- Membership in BDVA (Big Data Value Association) and EUDAT CDI
- Foundation of e-INFRA CZ
- Launch of the LEXIS project, coordinated by IT4Innovations

2020
- Establishment of the Digital Innovation Hub Ostrava
- IT4Innovations becomes the National Competence Centre in HPC

2021
- Launch of the Karolina supercomputer
- Termination of operating the Anselm and Salomon supercomputers
- Membership in the EOSC Association

2022
- Foundation of the European Digital Innovation Hub Ostrava (EDIH Ostrava)

2023
- IT4Innovations joins the iRODS consortium
- Completion of the complementary systems' installation
- Start of the EXA4MIND project, coordinated by IT4Innovations
- IT4Innovations becomes part of the MaX and SPACE Centres of Excellence

2024
- Contract signed for the delivery of the VLQ quantum computer of the LUMI-Q consortium
- IT4Innovations becomes part of the POP3 and CLARA Centres of Excellence
- Membership in VI-HPS and WHPC

Mission, Vision, and Memberships

Mission

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

Vision

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

Memberships

IT4Innovations actively participates in the EuroHPC Joint Undertaking activities and is a member of critical European infrastructures, initiatives, and associations in HPC, HPDA, AI, and QC. 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
- VI-HPS – Virtual Institute – High Productivity Supercomputing
- WHPC – Women in High Performance Computing

Organisational Structure IT4Innovations

IT4Innovations Management

Managing Director | Doc. Vít Vondrák

Scientific Director | Prof. Tomáš Kozubek

- → Advanced Data Analysis and Simulations Lab | Dr Jan Martinovič
- → Infrastructure Research Lab | Doc. Lubomír Říha
- → Parallel Algorithms Research Lab | Dr Tomáš Karásek
- → Modelling for Nanotechnologies Lab | Prof. Michal Otyepka
- → Quantum Computing Lab | Prof. Marek Lampart
- → Training and Education | Karina Pešatová

Supercomputing Services Director | Dr Branislav Jansík

- → HPC Operations and Administration | Radovan Pasek
- → User Support | Petra Lyčková Navrátilová

- → Communications | Zuzana Červenková
- → Public Procurement and Legal Service | Jan Juřena
- → Finance | Petr Válek
- → Administrations and Operations | Helena Starková
- → Development | Martin Duda

Scientific Council of IT4Innovations

Chairman | Doc. Vít Vondrák

Internal Members

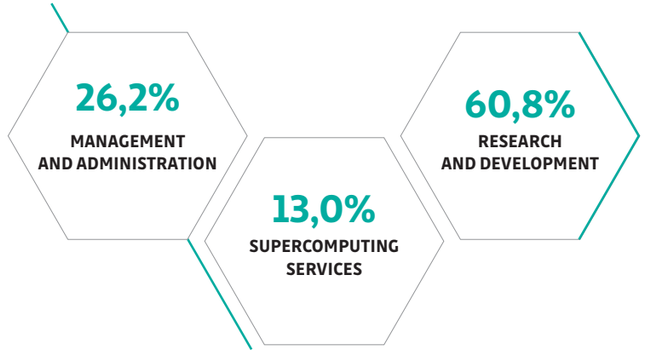
- → Prof. Tomáš Kozubek
- → Dr Branislav Jansík
- → Dr Jan Martinovič
- → Doc. Lubomír Říha
- → Dr Tomáš Karásek
- → Prof. Michal Otyepka
- → Prof. Marek Lampart

External Members

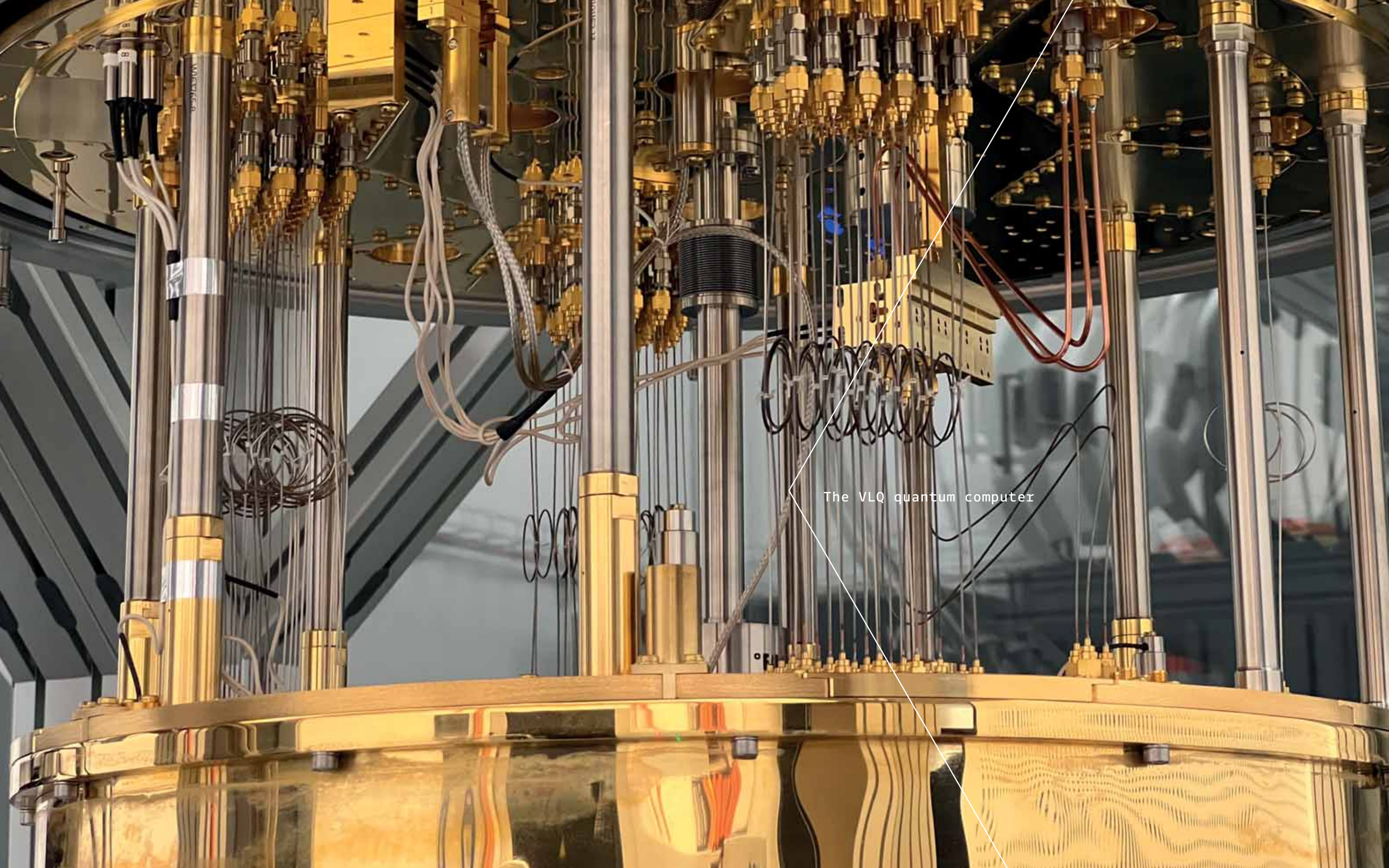
- → Prof. Jiří Damborský | Loschmidt laboratories of Masaryk University Brno
- → Prof. Jiří Jaroš | Faculty of Information Technology, Brno University of Technology
- → Dr Jakub Šístek | Institute of Mathematics of the Czech Academy of Sciences
- → Doc. Pavel Jelínek | Institute of Physics of the Czech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

Employees of IT4Innovations

In 2024, the number of IT4Innovations employees converted to full-time eqivalent (FTEs) totalled 154,32 FTEs, of which:



- 40,0% Advanced Data Analysis and Simulations Lab
- 19,1% Infrastructure Research Lab
- 14,9% Parallel Algorithms Research Lab
- 19,8% Modelling for Nanotechnologies Lab
- 6,2% Big Data Analysis Lab



The VLQ quantum computer

02
IMPORTANT EVENTS

January

- The cover of **ChemPhysChem** featured an illustration from research conducted by IT4Innovations, the Faculty of Electrical Engineering and Computer Science at VSB-TUO, and Université Toulouse III.
- Start of the third phase of the POP project (**POP3**) within the Centre of Excellence focused on performance optimisation and productivity. The project will focus on flagship European HPC applications developed in other Centres of Excellence while continuing to provide services to HPC users and SMEs.
- Launch of the **FALCON** project, in which IT4Innovations is a consortium member. The project aims to improve the competitiveness of the European aerospace industry by focusing on fluid–structure interaction phenomena to improve aircraft aerodynamics.
- IT4Innovations joined the **AVITHRAPID** project, aiming to support the search for new broad-spectrum antiviral compounds by developing various methods.

February

- Launch of the **EPICURE** project, which will operate an HPC application support service for European scientists and researchers. IT4Innovations is one of the project partners.

March

- VSB – Technical University of Ostrava, including IT4Innovations, in cooperation with the University of Ostrava and other partners, fully launched the **REFRESH** project to address regional challenges and contribute to its economic, energy, and environmental transformation.

April

- Co-organisation of the **NanoLumCat** workshop, one of the world's largest meetings focused on carbon dots and single-atom catalysis for renewable energy sources.
- The **Karolina** supercomputer underwent a software update that was necessary to ensure compatibility with new versions of tools and applications. The update essentially meant a complete reinstallation of the supercomputer.

May

- IT4Innovations and its partners in the EVEREST project released a set of open-source development tools. The **EVEREST SDK** integrates tools to simplify deploying applications on heterogeneous high-performance cloud infrastructures, especially those offering FPGA acceleration.
- IT4Innovations organised the 6th edition of the **HPCSE** conference, attracting experts not only from applied mathematics, numerical analysis, data analysis, machine learning, and advanced visualisation but also from quantum computing.

June

- The **Journal of the American Chemical Society** featured on its cover a joint study by researchers from CATRIN of Palacký University in Olomouc, CEET, and IT4Innovations of VSB-TUO, describing a new way to influence fluorographene properties using UV light.
- IT4Innovations deployed the **NVIDIA CUDA Quantum simulator** on the Karolina and Barbora supercomputers, enabling hybrid application development and significantly enhancing productivity and scalability in quantum computations.

July

- In collaboration with the International Clinical Research Center and Masaryk University, IT4Innovations launched the new **AggreProt** web server, designed to predict protein aggregation.

Augustt

- Researchers from IT4Innovations developed a **new method for optimising the performance of finite element method** (FEM) computations. Their innovative adaptive solution, which adjusts the calculations based on the parameter set during runtime, achieves up to an eightfold speed-up.
- A new generation of supercomputing experts was trained at the **HPC in Data Science summer school**, organised by IT4Innovations as part of the EUMaster4HPC project. The summer school focused on data science using supercomputing and was attended by more than 40 students from all over Europe.

September

- A contract for the acquisition of the **VLQ quantum computer** of the LUMI-Q consortium was signed. It will be installed at IT4Innovations as part of an agreement between the EuroHPC Joint Undertaking and IQM Quantum Computers, which won the selection procedure as the supplier.
- IT4Innovations co-organised the international **PPAM** conference, which was attended by Turing Award laureate **Jack Dongarra** from the University of Tennessee and Oak Ridge National Laboratory, as well as **Satoshi Matsuoka**, Director of the RIKEN Center for Computational Science.
- As part of the LIGATE project, breakthrough **LIGEN** computations were demonstrated, running in parallel on the LUMI, Karolina, Leonardo, and E4 supercomputers. These computations were launched via the LEXIS Platform 2 portal using the HEAppE framework, and the calculations themselves were carried out using the HyperQueue tool, developed over the long term at IT4Innovations.
- During the European **Researchers' Night**, 730 visitors discovered the "secrets of supercomputers" at IT4Innovations.

October

- Publication of the **Industry 4.0: The Foundation of the Economic Transformation of the Czech Republic** book by Vladimír Mařík, Robert Keil, and colleagues, co-authored by Vít Vondrák, Marek Lampart, Michal Podhorányi, Kateřina Slaninová, and Ivan Zelinka from IT4Innovations.

November

- Establishment of the unique, interdisciplinary **CLARA Centre of Excellence** in the Czech Republic, which focuses on developing a new generation of applications using AI, computational modelling, and quantum computing. The consortium, which includes IT4Innovations, aims to advance research into neurodegenerative diseases, especially Alzheimer's disease.

- IT4Innovations joined the international **VI-HPS** initiative to increase productivity in supercomputing applications.
- The **8th Users' Conference of IT4Innovations** was attended by 79 participants.
- IT4Innovations established cooperation with **Argonne National Laboratory** in the field of scientific data visualisation and with **Oak Ridge National Laboratory** as part of the ExaDigit initiative, focused on digital twins of data centres and HPC infrastructure.

December

- In Luxembourg, results were announced for the European AI Factories call, supporting the wider deployment of AI tools across society and industry in Europe. One of the winning projects was **LUMI AI Factory**, which builds on the successful LUMI consortium, operating one of the most powerful European supercomputers, in which the Czech Republic participates represented by IT4Innovations.
- IT4Innovations will participate in implementing and operating the **Federation Platform** for the EuroHPC Joint Undertaking.
- IT4Innovations co-founded the Central European Chapter of the global **Women in High Performance Computing** organisation.
- Publication of **Strategic Research Agenda 6**, mapping the current European HPC, AI, and quantum computing ecosystem. IT4Innovations experts contributed to its creation and related White Papers.

03
FINANCIAL REVIEW

IT4Innovations Economic Balance

The total expenditures of IT4Innovations amounted to CZK 295,470,000 in 2024. Of this amount, operating (non-investment) and investment (capital) expenditures accounted for 97.9% and 2.1%, respectively.

Operating expenditures amounted to CZK 289 million. The largest share of these expenditures consisted of personnel costs, services (including electricity consumption costs, maintenance of operated systems and supporting infrastructure, technical and system support, etc.), and overheads.

Investment expenditures amounted to CZK 6 million in 2024, covering, among other things, the acquisition of virtualisation infrastructure, an NVIDIA Grace CPU Superchip server, and costs related to the preparation for modernising the data room cooling system.

In 2024, a pre-tax profit of CZK 6,143,000 was achieved.

IT4Innovations Economic Balance

A. Operational expenditures	Personnel costs – research teams	CZK 103,848,000
	Personnel costs – management and administration	CZK 43,934,000
	Personnel costs – supercomputing services	CZK 22,463,000
	Services	CZK 60,731,000
	Overheads	CZK 42,277,000
	Domestic and international business trips	CZK 9,554,000
	Fees	CZK 1,633,000
	Minor long-term tangible assets	CZK 1,630,000
	Consumables	CZK 1,227,000
	Other costs	CZK 1,178,000
	Scholarships	CZK 789,000
	Total operational expenditures	**CZK 289,264,000**
B. Investment expenditures	Long-term tangible assets – machines and equipment	CZK 4,795,000
	Long-term tangible assets – buildings	CZK 1,411,000
	Total investment expenditures	**CZK 6,206,000**
C.	**Total expenditures** (A.+ B.)	**CZK 295,470,000**
D.	**Total sources of funding**	**CZK 301,613,000**
E.	**Balance total** (D.- C.)	**CZK 6,143,000**

Sources of Funding

In 2024, IT4Innovations' overall budget was CZK 301,613,000. National grants and international grants accounted for the largest share of funding sources, followed by internal resources (operating fund and contribution to educational activities).

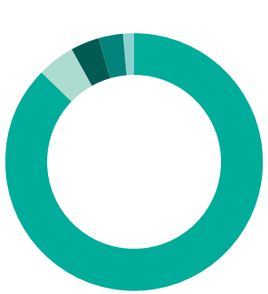
Sources of funding for the institutes' costs

CZK 301,613,000 in total

46,0%	National grants
20,7%	International grants
18,6%	Internal resources
7,6%	European structural and investment funds
2,5%	Long-term research organisation development fund
2,5%	Contract research and rental of computational resources
2,1%	Other

National grants

CZK 138,775,000 in total



87,3%	Ministry of Education, Youth and Sports of the Czech Republic
4,8%	Czech Science Foundation
3,6%	Technology Agency of the Czech Republic
3,0%	Ministry of the Interior of the Czech Republic
1,3%	Moravian-Silesian Region

European structural and investment funds

CZK 22,773,000 in total

52,4%	Operational Programme Johannes Amos Comenius
40,3%	Operational Programme Just Transition
7,3%	Operational Programme Technologies and Application for Competitiveness

International grants

CZK 62,414,000 in total

22,5%	EUROCC2
13,0%	EXA4MIND
7,8%	POP3
7,6%	BioDT
7,2%	EDIH Ostrava
5,2%	SPACE
4,9%	MAX
4,1%	OpenWebSearch.EU
4,1%	FALCON
3,8%	EPICURE
3,0%	EUPEX
2,5%	EUMaster4HPC
2,4%	ACROSS
2,2%	LIGATE
2,0%	EVEREST
1,9%	TWIN SYNERGIES
1,6%	DTO-BioFlow
1,4%	IO-SEA
0,6%	AVITHRAPID
0,5%	Superheroes 4 Science
0,4%	CZQCI
0,4%	SCALABLE
0,3%	s-NEBULA
0,2%	CLARA
0,2%	EOSC-ENTRUST
0,1%	SCtrain
0,1%	Other (PRACE 6IP, Circulight, DICE, OPENQKD)

04
LIST OF PROJECTS

National projects

Projects supported by the Ministry of Education, Youth and Sports

Large Infrastructure for Research, Experimental Development and Innovation Project
- e-Infrastructure CZ

Projects of the Operational Programme Johannes Amos Comenius
- e-INFRA CZ Modernisation II
- European Open Science Cloud Czech Republic
- National Repository Platform for Research Data

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

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

Projects supported by the Czech Science Foundation

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

Postdoc individual fellowship – incoming
- Magnetoelasticity of non-cubic materials in spin-lattice dynamic simulations

Projects supported by the Technology Agency of the Czech Republic

M-ERA.NET Programme
- Flexible manufacturing approach for recyclable bio-based high performance composite molds

TREND Programme
- Optimization of design and production processes of vertical pumps using modern technologies

Projects supported by the Ministry of Industry and Trade

Operational Programme Technologies and Applications for Competitiveness
- Terahertz and Raman optical activity spectrometers with extended application possibilities
- EyeERP – complex ERP system for eye clinics with mobile application MojeOči for performing and AI analysis of eye tests
- Advanced medical data visualization with AI support

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

- Research on holistic model of interconnected critical electricity and communication infrastructures

VSB-TUO Projects with IT4Innovations Participation

- REFRESH – Research Excellence For REgion Sustainability and High-tech Industries
- Validation of integrating artificial intelligence for receiving emergency calls
- Center of Energy and Environmental Technologies
- Combination of holographic and digital safety protection
- National Centre for Energy II

International projects

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

- LIGATE – LIgand Generator and portable drug discovery platform AT Exascale
- EUMaster4HPC – European Master for High Performance Computing
- EVEREST – dEsign enVironmEnt foR Extreme-Scale big data analyTics on heterogeneous platforms
- ACROSS – HPC big dAta artifiCial intelligence cross stack platfoRm tOwardS exaScale
- IO-SEA – IO Software for Exascale Architecture
- EUPEX – European Pilot for 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
- OpenWebSearch.EU – Piloting a Cooperative Open Web Search Infrastructure to Support Europe's Digital Sovereignty
- EXA4MIND – EXtreme Analytics for MINing Data spaces
- SPACE – Scalable Parallel and distributed Astrophysical Codes for Exascale
- MaX – MAterials design at the eXascale
- DTO-BioFlow – Integration of biodiversity monitoring data into the Digital Twin Ocean
- FALCON – Foreseeing the next generation of Aircraft
- POP3 – Performance Optimisation and Productivity 3
- AVITHRAPID – Antiviral Therapeutics for Rapid Response Against Pandemic Infectious Diseases
- CLARA – Center for Artificial Intelligence and Quantum Computing in System Brain Research
- EOSC-ENTRUST: A European Network of TRUSTed research environments
- TWIN SYNERGIES – Empowering participation and accelerating synergies in Widening countries with a focus on Green & Digital Transition

Digital Europe Programme

- EUROCC 2 – National Competence Centres in the Framework of EuroHPC Phase 2
- CZQCI – Czech National Quantum Communication Infrastructure
- EDIH Ostrava – European Digital Innovation Hub Ostrava
- EPICURE – High-level specialised application support service in High-Performance Computing

International Visegrad Fund

- Superheroes 4 Science

The Karolina supercomputer

05

SUPERCOMPUTING SERVICES

IT4Innovations operates the most powerful supercomputing systems in the Czech Republic, primarily serving academic institutions and research 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 2024, IT4Innovations operated two supercomputers — Karolina (15.7 PFlop/s) and **Barbora** (849 TFlop/s). The petascale **Karolina** system was fully commissioned in summer 2021. It was acquired under the EuroHPC Joint Undertaking, with 35% of its computing capacity available to users from EuroHPC JU member states. Immediately after its launch, Karolina ranked among the most powerful supercomputers in Europe. In the TOP500 List, which assesses supercomputers by performance, it was placed 69th worldwide and 19th in Europe at the time of its launch. In the Green500 List of the most energy-efficient supercomputers, it achieved 8th place globally and third place in Europe.

In 2024, the Karolina supercomputer underwent a **software upgrade** necessary to ensure compatibility with new versions of tools and applications, which essentially meant reinstalling the entire system.

Two fully functional cloud environments, created from Karolina's cloud nodes, were made available to IT4Innovations computational resource users with active projects. Specifically, the **e-INFRA CZ Cloud** is intended for users of the e-INFRA CZ infrastructure, while the **IT4I Cloud** serves other users.

Thanks to IT4Innovations' membership in the LUMI consortium, composed of eleven European countries, Czech researchers can use one of the world's most powerful and modern supercomputers – **LUMI**. Fully operational since 2023, LUMI offers a theoretical peak performance of 531.5 PFlop/s. IT4Innovations is part of its management structure, provides expert support to users through the LUST (LUMI User Support Team), participates in its operation, and develops software tools such as HyperQueue, which allows users to efficiently utilise the available computational resources of LUMI.

In 2024, LUMI's computational resources were allocated to **80 projects** via Open Access Grant Competitions of IT4Innovations, with a total volume reaching nearly 850,000 node hours.

**For evaluating the use of IT4Innovations computational resources, we rely on the concept of node hours, as computer clusters and individual nodes differ in architecture and performance. Each computing system has specific parameters, such as processor types, GPU accelerators, and other factors influencing its performance. Although these node hours are summed across different computer clusters for simplification purposes, they do not reflect differences in the performance of individual compute nodes.*

Complementary systems

In 2022 and 2023, IT4Innovations installed systems composed of various hardware platforms, allowing access to emerging, non-traditional, or highly specialised architectures. The latest addition is a server equipped with the **NVIDIA Grace CPU Superchip**, featuring two processors, each with 72 Arm Neoverse V2 cores. This architecture, together with fast LPDDR5X memory, represents the current trend in HPC. The same type of processor is also used in Europe's first exascale JUPITER supercomputer , installed in Jülich, Germany.

PROJECT data storage

The IT4Innovations data room also houses a large-capacity data storage system called PROJECT, which stores and backs up data processed or generated on IT4Innovations' supercomputers. The **PROJECT data storage** is a central storage for both IT4Innovations project and user data. For each active project, a dedicated project directory is created, whose lifecycle strictly mirrors the project's lifecycle. The total storage capacity is 15 PB.

VLQ quantum computer

In 2024, the EuroHPC JU signed a contract with the IQM Quantum Computers company for the delivery of the **VLQ quantum computer**, which will be installed and operated at IT4Innovations. This 24-qubit system, based on superconducting qubits in a star topology, minimises swap operations, enabling more efficient execution of complex quantum algorithms.

VLQ will be integrated with the Karolina supercomputer and will become the first Czech quantum computer. It will be available to researchers, industry, and the public sector, expanding Europe's computing infrastructure with new technologies of significant industrial, scientific, and societal importance for Europe.

Technical Specifications of the Supercomputers

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

The Karolina supercomputer

Computational Resource Allocation

Computing time

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

Computing time on IT4Innovations supercomputers can be acquired in the following ways:

- **Open Access:** IT4Innovations computational resources are allocated to the Czech research community based on scientific excellence, computational competence, readiness, and societal and economic impact. The largest share of computing time is allocated through **Open Access Grant Competitions**, which are announced three times a year. Other options include **Institutional and Community Access**, supporting specific research, development, and innovation activities of selected research organisations, as well as **Fast Track Access**, intended for short-term tasks and application testing.
- **Access to Thematic HPC Resource Utilisation:** Computational resources are provided for socially significant projects, teaching and education, commercial use, and research on the infrastructure itself. Applications can be submitted at any time.

Within both approaches, computing time can be obtained on the Karolina and Barbora supercomputers, as well as on the Finnish LUMI supercomputer , where extensive GPU resources are available to employees of Czech research organisations.

- **EuroHPC JU Grant Calls:** The EuroHPC Joint Undertaking regularly announces open calls offering 35% of the capacity of petascale systems and up to 50% of the capacity of pre-exascale systems. This also applies to the Czech Karolina supercomputer, where 35% of the capacity is reserved for projects submitted through these calls. For the Finnish LUMI supercomputer, it is 50% of its total capacity.

Distribution of computational resources in 2024

- 83% Open Access projects
  5,511,051 of used node hours*
- 16% EuroHPC JU Grant Competitions
  1,059,391 of used node hours*
- 1% Access to Thematic HPC Resource Utilisation, including the rental of computational resources
  84,174 of used node hours*

From 2013 to the end of 2024, IT4Innovations' computational resources were used for **2,443 projects** across various scientific fields. These projects covered a wide range of disciplines – from the development of new materials and drugs, through engineering tasks, to scientific data visualisation. In recent years, the focus has increasingly shifted towards machine learning, artificial intelligence, and quantum algorithm research.

In 2024, there were **627 active projects**, which together consumed **6,654,617 node hours** of computing time.

** The consumed node hours provide an indication of the actual amount of computing time used in 2024. The total value here comprises all projects that actually ran in 2024 on the Karolina and Barbora supercomputers and the NVIDIA DGX-2 system at IT4Innovations. On the LUMI supercomputer, computational resources were allocated under open access to 80 projects, totalling 844,765 node hours.*

Open Access / Open Access Grant Competitions

In 2024, three Open Access Grant Competitions were announced, supporting a total of **176 research projects**, including 19 multi-year projects. Specifically, these were the 30th, 31st, and 32nd calls.

According to the schedule of each call, successful applicants were granted computational resources during 2024. For standard projects, computational resources are provided for a period of 12 months, while for multi-year projects, they are granted for 24 or 36 months, to support long-term research projects.

In these three Open Access Grant Competitions, applicants applied for almost 9 million node hours. The demand for computational resources exceeded the resources offered; therefore, the allocation committee decided to reduce the allocations for the evaluated projects. In total, **6.49 million node hours** were distributed across 176 projects within these calls on the Karolina, Barbora, and LUMI supercomputers.

Projects in the field of materials science received the most computational resources. Physics and astronomy projects ranked second, followed by computer science projects.

By institution, scientists from VSB – Technical University of Ostrava received the highest allocations for their projects. The Czech Academy of Sciences ranked second, and Charles University third.

The largest number of projects awarded computational resources were submitted by researchers from VSB – Technical University of Ostrava, the Czech Technical University in Prague, and various institutes of the Czech Academy of Sciences.

Researchers from ten different institutes of the Czech Academy of Sciences received computational resources for a total of 28 projects. Among the institutes making the greatest use of IT4Innovations infrastructure – as in previous years – were the Institute of Organic Chemistry and Biochemistry, the Institute of Plasma Physics, the J. Heyrovský Institute of Physical Chemistry, and the Institute of Physics.

In 2024, researchers could also utilise 115,007 node hours on the accelerated part of the **LUMI** supercomputer, which had been allocated through a **special call** announced at the end of 2023. Nine projects focused on artificial intelligence, mainly from the Czech Technical University in Prague and the Technical University of Liberec, gained access to these computational resources until November 2024. The call targeted socially significant tasks, especially AI applications and projects using GPU acceleration.

Computational resources allocated within the Open Access Grant Competitions in 2024 by scientific discipline

55%	Materials science (73 projects)
17%	Physics and astronomy (24 projects)
10%	Computer science (30 projects)
9%	Biosciences (27 projects)
6%	Engineering (8 projects)
2%	Earth sciences (6 projects)
1%	Applied mathematics (8 projects)

Computational resources allocated in Open Access Grant Competitions in 2024 by institutions

31%	VSB – Technical University of Ostrava (35 projects)
18%	Czech Academy of Sciences (30 projects)
15%	Charles University (22 projects)
9%	Czech Technical University in Prague (32 projects)
6%	University of South Bohemia in České Budějovice (3 projects)
5%	University of Ostrava (8 projects))
4%	University of Chemistry and Technology, Prague (5 projects)
2%	Masaryk University (9 projects)
2%	Palacký University Olomouc (8 projects)
2%	University of West Bohemia in Pilsen (4 projects)
2%	Brno University of Technology (11 projects)
2%	CEITEC (2 projects)
1%	ELI-Beamlines (2 projects)
1%	Others (University of Pardubice, Silesian University in Opava, University Hospital Hradec Králové, Czech Aerospace Research Centre; 5 projects in total)

Computational resources consumed in 2024

Open Access

The computational resources consumed within Open Access Grant Competitions amounted to **5,436,909 node hours**. Within Fast Track Access, the primary aim of which is to prepare for grant competitions, **47,172 node hours** were consumed.

Thematic Capacity Access

In 2024, **11,563 node hours** were used for socially important tasks, training and educational activities, and in-house infrastructure research.

The computational resources provided through paid rental amounted to **72,611 node hours**. These were commercial projects for companies such as AIRMOBIS, DHI, Glass Service, and Varroc Lighting.

EuroHPC JU Grant Competitions

In 2024, **1,208,089 node hours** were provided on the Karolina supercomputer, shared among **106 projects** from **23 different countries**.

Most of the projects were from Austrian organisations, with researchers from Johannes Kepler University Linz participating in 13 projects. In other organisations, the number of projects ranged from 1 to 4 per organisation.

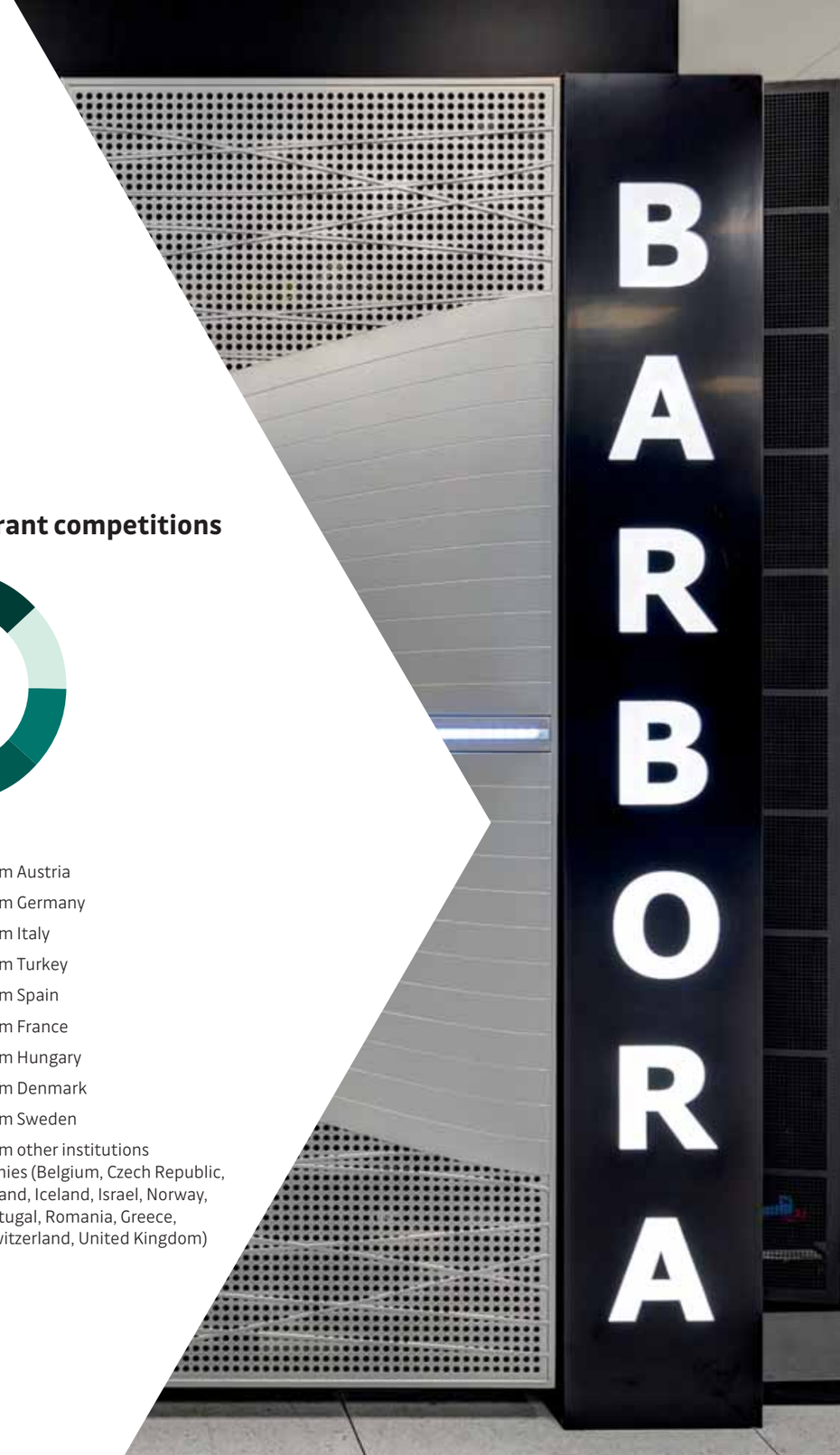
Users of computational resources

The number of active users of the IT4Innovations computing infrastructure increased year-on-year by 26% in 2024, reaching **2,632**.

The IT4Innovations Technical Support received a total of **2,062 queries and requests** in 2024. The internal response time (first reply within 24 hours) was met in 99.98% of cases. The internal closure time (not to exceed 30 days) was met in 99.23% of the queries.

EuroHPC JU grant competitions

- 14 projects from Austria
- 13 projects from Germany
- 12 projects from Italy
- 8 projects from Turkey
- 8 projects from Spain
- 6 projects from France
- 5 projects from Hungary
- 5 projects from Denmark
- 4 projects from Sweden
- 31 projects from other institutions and companies (Belgium, Czech Republic, Croatia, Ireland, Iceland, Israel, Norway, Poland, Portugal, Romania, Greece, Slovakia, Switzerland, United Kingdom)



06

RESEARCH AND DEVELOPMENT

IT4Innovations engages in excellent research primarily in the fields of high-performance computing (HPC), high-performance data analytics (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 connections. It is involved in all activities of the EuroHPC Joint Undertaking and participates in several key international infrastructures, initiatives, and associations (PRACE, ETP4HPC, EUDAT, BDVA, EOSC, iRODS, VI-HPS, WHPC).

In 2024, it was involved in **23 international projects** funded by the Horizon 2020, Horizon Europe, and Digital Europe programmes, coordinating the EXA4MIND and EDIH Ostrava projects. IT4Innovations is a member of the MaX, SPACE, POP3, and CLARA Centres of Excellence.

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

IT4Innovations has collaborated with the European Space Agency (ESA) since 2015. In 2024, it successfully completed the AIOPEN project in cooperation with Space Applications Services, Telespazio, KP Labs, and SERCO. Within this project, IT4Innovations focused on detecting urban changes using transformer architecture.

In 2024, IT4Innovations researchers published their results in 300 peer-reviewed journal publications such as Jimp and JSC, mostly in Q1 and Q2 journals.

IT4Innovations' research activities were carried out across five research labs:

- Advanced Data Analysis and Simulations Lab
- Infrastructure Research Lab
- Parallel Algorithms Research Lab
- Modelling for Nanotechnologies Lab
- Quantum Computing Lab

The IT4Innovations research labs obtained computational resources for **26 research projects** within the 30th to 32nd Open Access Grant Competitions. These projects received **nearly 2 million node hours**, representing approximately 30% of the total allocation for all supported projects. The highest number of projects (17) were submitted by researchers from the Modelling for Nanotechnologies Lab, which also received the largest share of computational resources — more than 1 million node hours. An additional 800,000 node hours were awarded to projects from the Infrastructure Research Lab and the Parallel Algorithms Research Lab.

Summary of Research and Development Results in 2024

Results classified based on the RIV 2017+

Summary of the achieved IT4Innovations research and development results in 2024

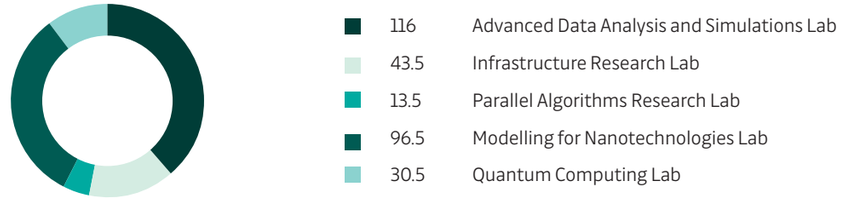
Results classified based on the RIV 2017+ Methodology	Achieved results
Jimp	258
JSC	42
Jost	6
B – reviewed publication	0
C – chapter in a reviewed publication	1
D – section in a proceeding	21
P – patent	0
F – utility model, industrial design	0
Z – semi-operation, verified technology	0
G – prototype, functional sample	0
H – results reflected in norms and directives	0
N – methodology, specialised map	0
R – software	16
V – research report	1

Jimp and JSC Journal Publications in 2024 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	27	36	43	8	2	116
Infrastructure Research Lab	9	10.5*	22	1	1	43.5
Parallel Algorithms Research Lab	1.5*	7.5*	3.5*	1	0	13.5
Modelling for Nanotechnologies Lab	42	34	19.5*	0	1	96.5
Quantum Computing Lab	8.5*	12	8	2	0	30.5
Total	88	100	96	12	4	300

**Articles shared among labs*

Number of journal publications in 2024 by individual research labs



List of D1 publications sorted by individual research labs

D1

Advanced Data Analysis and Simulations Lab

- Riaz M. B., Hussain A., Saddiqa A., Jarad F.: ***Numerical evaluation for the peristaltic flow in the proximity of double-diffusive convection of non-Newtonian nanofluid under the MHD.*** International Journal of Thermofluids. Volume 23, Issue August. 2024. DOI: 10.1016/j.ijft.2024.100791. D1
- Wiesner D., Suk J., Dummer S., Nečasová T., Ulman V., Svoboda D., Wolterink J. M.: ***Generative modeling of living cells with SO(3)-equivariant implicit neural representations.*** Medical Image Analysis. volume 91, Issue January, 2024. DOI: 10.1016/j.media.2023.102991. D1, IF 10.7
- Saleem S., Ahmad B., Naseem A., Riaz M.B., Abbas T.: ***Mono and hybrid nanofluid analysis over shrinking surface with thermal radiation: A numerical approach.*** Case Studies in Thermal Engineering. Volume 54, Issue February, 2024. DOI: 10.1016/j.csite.2024.104023. D1, IF 6.4
- Ishaq M., Rehman S.U., Riaz M.B., Zahid M.: ***Hydrodynamical study of couple stress fluid flow in a linearly permeable rectangular channel subject to Darcy porous medium and no-slip boundary conditions.*** Alexandria Engineering Journal. Volume 91, Issue March, p.50-69. 2024. DOI: 10.1016/j.aej.2024.01.066. D1, IF 6.2
- Faridi W.A., I., Riaz M.B., AlQahtani S. A., Wazwaz A.M.: ***The fractional soliton solutions of dynamical system arising in plasma physics: The comparative analysis.*** Alexandria Engineering Journal. Volume 95, Issue May; p.247-261. 2024. DOI: 10.1016/j.aej.2024.03.061. D1, IF 6.2
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- Jhangeer A., Ansari A. R., Imran M., Beenish, Riaz M.B.: ***Conserved quantities and sensitivity analysis influence of damping effect in ferrites materials.*** Alexandria Engineering Journal. Volume 86, Issue January, p.298–310. 2024. DOI: 10.1016/j.aej.2023.11.067. D1, IF 6.2
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- Ullah N., Rehman H. U., Asjad M.I., ; Riaz M.B., Muhammad Ta.: ***Wave analysis in generalized fractional Tzitzéica-type nonlinear PDEs: Contributions to nonlinear sciences.*** Alexandria Engineering Journal. Volume 92, Issue April, p.102-116. 2024. DOI: 10.1016/j.aej.2024.02.045. D1, IF 6.2
- Chan C.K., Riaz M.B., Rehman A.U., Ewe L.C., Sarwar L.: ***Dynamics of Jeffrey fluid flow and heat transfer: A Prabhakar fractional operator approach.*** International Journal of Thermofluids. Volume 22, Issue May. 2024. DOI: 10.1016/j.ijft.2024.100709. D1
- Bilal S., Yasir M., Riaz M.B.: ***Thermal characteristics of Falkner-Skan flow of time-dependent Maxwell material with varying viscosity and thermal conductivity. International Journal of Thermofluids.*** Volume 24, Issue November. 2024. DOI: 10.1016/j.ijft.2024.100833. D1
- Hussain A., Riaz M.B., Dar M.N.R., Cheema W.K., Shflot A. S., Malik M. Y.: ***Unraveling the transformative impact of ternary hybrid nanoparticles on overlapped stenosis with electroosmotic vascular flow kinetics and heat transfer.*** Case Studies in Thermal Engineering. Volume 59, Issue July. 2024. DOI: 10.1016/j.csite.2024.104589. D1, IF 6.4
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- Bilal S., Yasir M., Riaz M.B.: ***Numerical heat transfer assessment for rheological aspects of nonlinear thermally radiative flow of tangent hyperbolic nanofluid.*** International Journal of Thermofluids. Volume 23, Issue 8. 2024. DOI: 10.1016/j.ijft.2024.100792. D1
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D1

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IT4I

The IT4Innovations Visualisation and Virtual Reality Lab

Infrastructure Research Lab

- Jhangeer A., Zahid A., Amjad Z., Raza N., Muhammad T.: ***Lax pairs and Bäcklund transformations for a new (3+1)-dimensional integrable equation utilizing symbolic computation.*** Ain Shams Engineering Journal. Volume 15, Issue 12. 2024. DOI: 10.1016/j.asej.2024.103085. D1, IF 6.0
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Parallel Algorithms Research Lab

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Results of the last evaluation based on the M1 module of the RIV 2017+ Methodology rated with grades 1–3

Advanced Data Analysis and Simulations Lab

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Infrastructure Research Lab and Parallel Algorithms Research Lab

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Modelling for Nanotechnologies Lab

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Advanced Data Analysis and Simulations Lab

Head of Lab: **Dr Jan Martinovič** / Number of employees **37.51 FTE**

The lab focuses on advanced data analysis, research, and development in the field of 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.

Significant activities:

- Launch of the AVITHRAPID project, aimed at developing a range of small-molecule antivirals that can be rapidly designed and used for treating infectious diseases.
- The lab, in collaboration with the International Clinical Research Center and Masaryk University, launched a new web server, AggreProt, for predicting protein aggregation.
- Continued development of the LEXIS platform, the HPC-as-a-Service interface HEAppE, the Floreon+ system, the HyperQueue scheduler, and the development of a voice assistant for emergency calls
- Completion and successful defence of the EuroHPC LIGATE, IO-SEA, and ACROSS projects, as well as the H2020 EVEREST project, including the successful evaluation of the Czech parts of the EuroHPC projects.
- The LIGATE project successfully demonstrated a comprehensive computational workflow for drug discovery, carried out through the LEXIS platform using four supercomputers simultaneously, thus validating the key features of this platform.
- Successful completion of activities carried out under the ESA-TEP 4 industrial contract and the AIOPEN project funded in cooperation with the European Space Agency.
- Launch of the EOSC ENTRUST project, which aims to create a network of secure research environments for working with sensitive data and to support Europe's interoperability through a shared framework for data access and analysis.
- Jan Martinovič became the leader of the Data Management working group for artificial intelligence and machine learning within the EOSC CZ initiative.
- Continued collaboration with Fondazione LINKS on the B-CRATOS project under an industrial contract.
- Collaboration with Apollo Data on the EyeERP project — a comprehensive ERP system for ophthalmology clinics with the mobile app MojeOči for performing and AI-based analysis of eye tests (funded under OP TAC).
- Completion of the Center of Energy and Environmental Technologies project, supported by the TA CR THÉTA programme, in which the lab contributed, for example, by developing interactive software.
- Organisation of 17 training activities under the EOSC Training Centre.
- Co-authorship of the Industry 4.0: The Foundation of the Economic Transformation of the Czech Republic publication by Vladimír Mařík, Robert Keil, and colleagues.

Infrastructure Research Lab

Head of Lab: **Doc. Lubomír Říha** / Number of employees: **17.91 FTE**

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

Significant activities:

- IT4Innovations became a partner in the EuroHPC Centre of Excellence focused on performance optimisation and productivity (POP3), which concentrates on analysing the performance and efficiency of HPC applications. The aim is to provide services to all computing system users and SMEs. Collaboration continues within the MaX (optimisation and development of HPC applications in materials science) and SPACE (optimisation and development of HPC applications for astrophysics and cosmology research) Centres of Excellence.
- The FALCON project was launched, aiming to increase the competitiveness of the European aerospace industry by improving aircraft aerodynamics. Airbus is among the project partners.
- The EPICURE project was launched to support users in optimising the deployment of their applications on supercomputers. The team provides support ranging from optimising the deployment of existing codes to code optimisation and porting to GPU accelerators.
- Collaboration began with EXELIZ Solutions under an industrial contract for deploying the comprehensive MERIC Energy Efficiency HPC SW Suite, developed at IT4Innovations, to monitor and control electricity consumption of HPC clusters on the Portuguese EuroHPC Deucalion system.
- The Advanced Visualisation of Medical Data Using AI project was launched, supported by the OP TAC (MIT CR), in collaboration with Misterine.
- Development of new LATEST (analysis of GPU accelerator behaviour) and SPACE Converter (processing and visualisation of large data sets from astrophysical simulations) software tools. Ongoing work on long-term tools such as MERIC, ESPRESO, and MESIO, as well as services on the IT4Innovations infrastructure like Medical as a Service and Rendering as a Service.
- Collaboration with the Fraunhofer Institute for Chemical Technology ICT on developing a new methodology for segmenting and evaluating diffusion coatings for steel surface treatment.
- Co-organisation of two workshops at the international PPAM24 conference – the first focused on RISC-V and the second on energy efficiency in HPC.
- Initiation of collaboration with Argonne National Laboratory in scientific data visualisation and with Oak Ridge National Laboratory within the ExaDigit initiative dedicated to digital twins of data centres and HPC infrastructure.
- Collaboration with the Faculty of Materials Science and Technology of VSB-TUO on the Integration of Holographic and Data Security Protection project, funded by TA CR.

Parallel Algorithms Research Lab

Head of Lab: **Dr Tomáš Karásek** / Number of employees: **13.97 FTE**

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.

Significant activities:

- Collaboration on the FALCON project, which aims to increase the competitiveness of the European aerospace industry by focusing on fluid-structure interaction phenomena during aircraft development to improve aerodynamics. Development of a hybrid surrogate model for fluid-structure interaction tasks.
- Collaboration with more than ten companies and start-ups from various sectors within the services of the National Competence Centre in HPC (EuroCC 2 project). Supercomputers contributed to accelerating innovation and development in healthcare, the automotive industry, glassmaking, manufacturing, energy, the rail industry, and materials development.
- Collaboration with the G-Team and Bellmer companies under industrial contracts. Provision of expert consulting for Porsche and implementation of a proof-of-concept with VALVEA.
- Consulting services for companies and assistance with preparing project proposals under the FFplus call funded by EuroHPC JU.
- Collaboration on the REFRESH project – development of automated simulation workflows and surrogate models for proton exchange membrane fuel cells.
- Long-term collaboration with Fraunhofer ICT and the launch of the Flexible Manufacturing Approach for Recyclable High-Performance Biobased Composite Moulds (FutureMold) joint project, supported by the TA CR SIGMA programme.
- Launch of the Optimisation of Design and Manufacturing Processes for Vertical Pumps Using Modern Technologies project, supported by the TA CR TREND programme.
- Within the European Digital Innovation Hub Ostrava (EDIH Ostrava), several sub-projects were implemented across different industries, focusing on solving specific industrial challenges using advanced computational modelling, simulations, and prototyping techniques.
- Anum Shafiq participated as an invited speaker and a member of the technical programme committee at the 8th International Conference on Mechanics, Mathematics and Applied Physics (ICMMAP 2024) in Dalian, China.

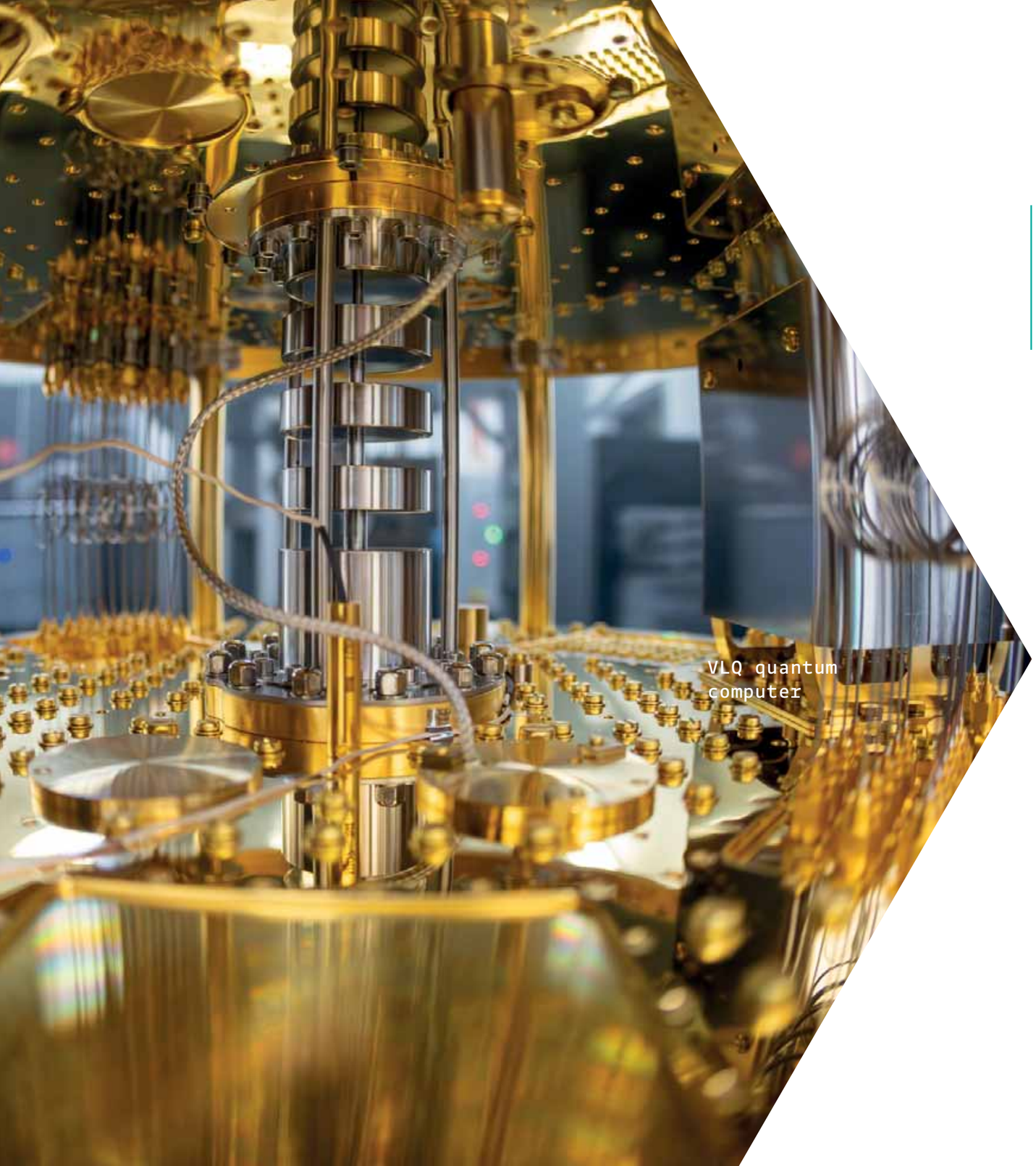
Modelling for Nanotechnologies Lab

Head of Lab: **Prof. Michal Otyepka** / Number of employees: **18.57 FTE**

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

Significant activities:

- A unique pathway for developing a new generation of antibiotics that are not only effective against a wide range of bacteria but can also reliably prevent the development of bacterial resistance was discovered by scientists from Palacký University Olomouc and VSB-TUO, in collaboration with colleagues from China.
- Implementation of the Experimental and theoretical studies of near-infrared-emitting and chiral carbon dot luminophores project, supported by the Global Experts programme of the Moravian-Silesian Region.
- Organisation of the NANOLUMCAT workshop under the auspices of the Global Experts programme.
- Collaboration on the international EXA4MIND project and national projects such as REFRESH (Ministry of the Environment of the Czech Republic), Influence of Thermoelectric Effects on Spin-Orbital Torques in 2D van der Waals Materials (Ministry of Education), and projects funded by the Czech Science Foundation – Magnetism at interfaces: from quantum to reality, Novel thermoelectric, thermovoltaic, and phonoelectric heat conversion systems based on nitrides semiconductors, Magnetoelasticity of non-cubic materials in spin-lattice dynamic simulations.
- The cover of the Journal of the American Chemical Society (JACS) featured a joint research project by scientists from CATRIN, Palacký University Olomouc, and VSB-TUO. Together, they discovered a new way to influence the properties of fluorographene using UV light.
- Completion of the Unconventional Superconductors under Extreme Conditions project, supported by the Czech Science Foundation. Experimentalists from Charles University and theorists from VSB-TUO collaborated on the research of the complex phase diagram of the UTe_2 compound and related compounds using a combination of experimental measurements and current theoretical ab initio calculations of thermal expansion, magnetostriction, heat capacity, magnetisation, elastic constants, and electrical transport of unconventional superconductors under multi-extreme conditions.



VLQ quantum computer

Quantum Computing Lab

Head of Lab: **Prof. Marek Lampart** / Number of employees: **5.81 FTE**

The lab focuses on developing new algorithms for quantum computers and simulators, including their practical applications, quantum error correction, research in quantum technologies, communication, cryptography, optimisation, and machine learning.

Significant activities:

- Installation of the NVIDIA CUDA Quantum simulator on the Barbora and Karolina supercomputers. On a single GPU of the Karolina supercomputer, it enables the simulation of 30 qubits.
- Collaboration on the international CZQCI – Czech National Quantum Communication Infrastructure (Digital Europe) project, the national REFRESH and Network Cybersecurity in Post-Quantum Era projects.
- Publication of the Industry 4.0: The Foundation of the Economic Transformation of the Czech Republic book by Vladimír Mařík, Robert Keil, and colleagues, co-authored by Vít Vondrák, Marek Lampart, Michal Podhorányi, Kateřina Slaninová, and Ivan Zelinka from IT4Innovations.
- Organisation of quantum computing training for ČEPS and the National Agency for Communication and Information Technologies.
- The laboratory organised a number of educational events, including seminars focused on quantum computing, which generated significant interest in 2024. A total of 254 participants attended these trainings.
- Paulina Lewandowska received the award for the Best PhD Thesis in Quantum Information defended in Poland, granted by the National Quantum Information Centre (KCIK, a research organisation comprising twelve Polish institutions), for her Validation Methods for Modern Quantum Architectures thesis.
- Presentation of the Quantum Computing Laboratory at the Global Quantum Symposium 2024, an interview for the Embassy of the Czech Republic in Bern, and representation at the Czech-Japan Workshop on Quantum Information in Tokyo, Japan.

07

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 2024, IT4Innovations organised **39 training courses, seminars, and workshops dedicated to HPC, HPDA, QC, AI,** and digital skills development as part of professional education.

Another 17 events were held within the **EOSC-CZ Training Centre**, where IT4Innovations coordinates the education of a broad scientific community in the Czech Republic on specialised topics in open science and FAIR data.

Educational Activities

Experts from IT4Innovations are actively involved in educational activities within PhD study programmes. The ongoing **Computational Sciences** PhD study programme guaranteed by IT4Innovations was attended by four students in 2024, three of whom successfully completed their studies. In other PhD study programmes guaranteed by the Faculty of Electrical Engineering and Computer Science of VSB-TUO, our colleagues acted as **supervisors** for six students in the Computational Sciences study programme and three students in the Informatics and Computational Sciences study programme.

In the **Computational and Applied Mathematics** MSc study programme, experts from IT4Innovations provide instruction in subjects focused on HPC. The programme is guaranteed by the Department of Applied Mathematics of the Faculty of Electrical Engineering and Computer Science of VSB-TUO. Students of this and other MSc study programmes are also offered the **Introduction to Quantum Computing** course. In 2024, the Faculty of Materials Science and Technology of VSB-TUO prepared the new **Computational Technologies in Materials Science** MSc study programme, in which IT4Innovations will provide instruction in several courses, for accreditation.

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 and research and supercomputing centres. The MSc study programmes started in the 2022 winter semester. In 2024, the first 18 students successfully completed their studies. Graduates are finding careers in fast-growing fields such as high-performance computing, advanced data analytics, and artificial intelligence. In 2024, IT4Innovations, in cooperation with the Vienna Scientific Cluster, a research centre of Vienna University of Technology, and MathWorks corporation, organised a summer school called **HPC in Data Science** for the students of the second cohort. It was attended by 40 first-year students from this study programme and 6 other MSc and PhD students from various European universities.

Training activities

IT4Innovations supports the Czech and international scientific community and its users by organising 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. IT4Innovations is also actively involved in raising awareness and developing knowledge in the areas of HPC, HPDA, AI, and quantum computing in the Czech Republic and abroad. The training activities are aimed at a wide range of participants from the academic environment and representatives of industrial and commercial entities interested in the effective use of advanced computing technologies.

The training activities are open to the European community through international projects in which IT4Innovations is involved, such as EuroCC 2, EPICURE, SPACE, POP and MaX Centres of Excellence, EDIH Ostrava, and others. Thematically, the courses offered by IT4Innovations focus on computer systems and their architecture, programming techniques and tools, libraries, and applications. Courses delivered by the EDIH Ostrava focus on developing digital skills for companies.

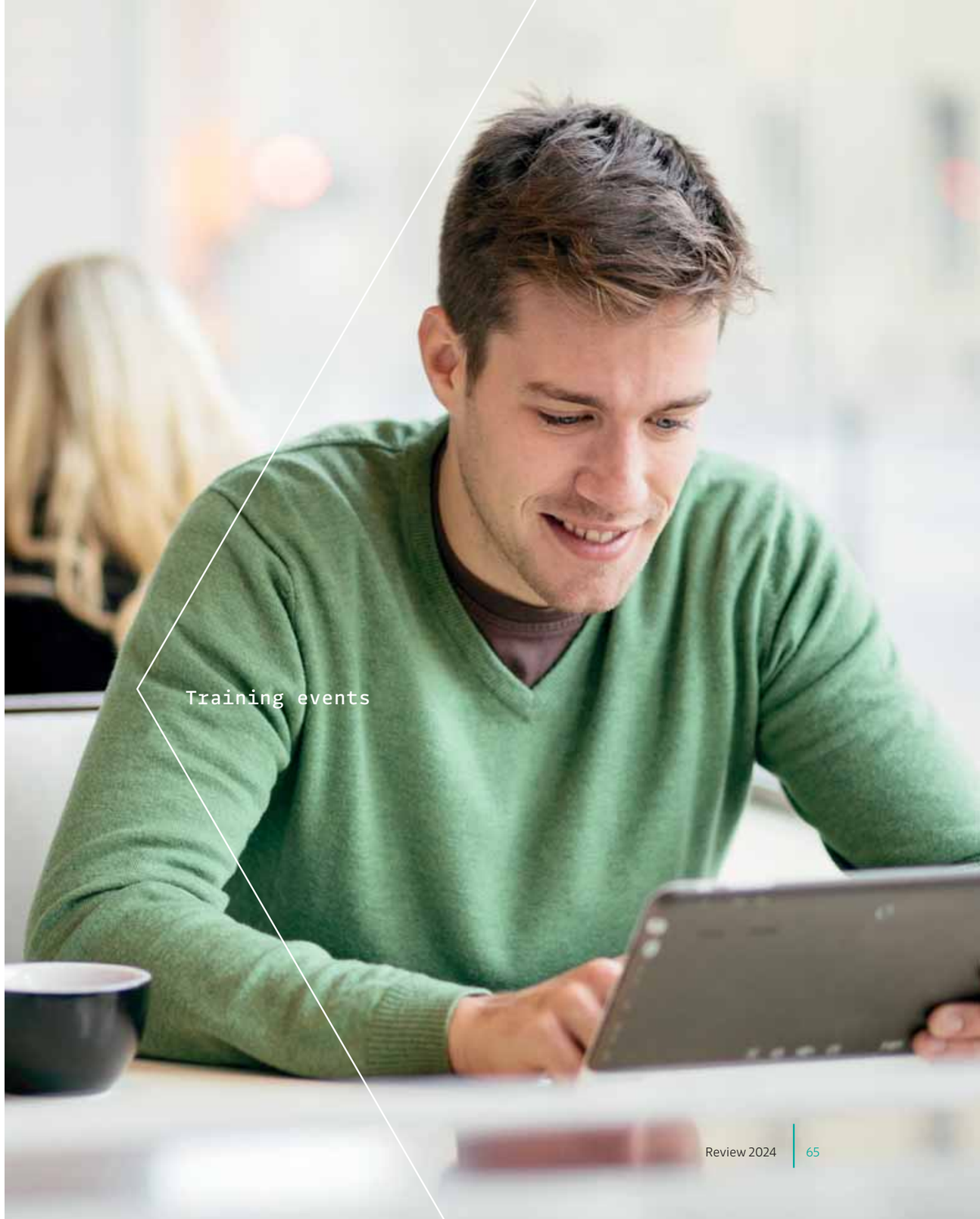
In 2024, IT4Innovations held **39 educational events,** attended by **886 participants,**whether in person or online.

Division of training courses by area

16	HPC
3	AI
13	QC
3	HPDA
4	Digital skills development

As part of the EOSC-CZ Training Centre, whose nationwide educational activities are coordinated by IT4Innovations, 17 events were held.

In 2024, IT4Innovations continued its cooperation with partners from Slovakia and Poland on the **Superheroes 4 Science** project, which is supported by the Visegrad Fund. The partners prepared entertaining interactive educational materials – comics, a computer game, a board game – and the content of two interactive workshops that introduce pupils, students, and the general public to the basic principles of quantum computing and artificial intelligence.



08
NATIONAL PROJECTS

Supercomputing Services Projects

→ **PROJECTS SUPPORTED BY THE MINISTRY OF EDUCATION, YOUTH AND SPORTS OF THE CZECH REPUBLIC**

Large Infrastructure 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 it 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 most powerful and advanced supercomputing systems in the Czech Republic, and high-capacity data storage.

Projects of the Operational Programme Johannes Amos Comenius

e-INFRA CZ II Modernisation (2023–2026)

- → Project ID: CZ.02.01.01/00/23_016/0008329
- → Principal Investigator: Doc. Vít Vondrák
- → The aim of the project is the modernisation and upgrade of the e-INFRA CZ e-infrastructure, which is a strategic infrastructure for research, development, and innovation in the Czech Republic. The modernisation focuses on specific components — 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
- → The European Open Science Cloud (EOSC) is a European initiative focused on developing infrastructure to support open science practices in research data management. It provides a framework for storing and making available so-called FAIR research data – findable, accessible, interoperable, and reusable. The EOSC-CZ project is the implementation of the EOSC initiative in the Czech Republic, aiming to create a national node of this European initiative and to promote best practices in research data management across scientific communities. As part of the implementation of the National Data Infrastructure (NDI), a common platform will be created for sharing, managing, and accessing data and computational resources for research purposes. The NDI will support both scientific and multidisciplinary research activities and will cover a wide range of scientific fields and disciplines.
- → www.eosc.cz

National Repository Platform for Research Data (2024–2028)

- → Project ID: CZ.02.01.01/00/23_014/0008787
- → Principal Investigator: Radovan Pasek
- → The National Repository Platform (NRP) will serve as a universal foundation for the effective handling of FAIR research data. The NRP comprises a secure system of technical and software tools that will provide sufficient capacity for storing data produced within state-supported projects and making it accessible. On top of this foundation, a system of services, tools, and methodological procedures will be available for the creation and long-term management of repositories and data stewardship in accordance with FAIR principles.

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.

→ PROJECTS SUPPORTED BY THE MORAVIAN-SILESIAN REGION

Global Experts Programme

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

- 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 CZECH SCIENCE FOUNDATION (GA CR)

International Grant Projects Evaluated on the LEAD Agency Principle

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

- 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

Unconventional superconductors under extreme conditions (2022–2024)

- Project ID: 22-22322S
- Principal Investigator: Dr Dominik Legut
- The project brings 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.

Novel thermoelectric, thermovoltaic, and phonoelectric 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.

Postdoc individual fellowship – incoming

Magnetoelasticity of non-cubic materials in spin-lattice dynamic simulations (2024-2026)

- Project ID: 24-11388I
- Principal Investigator: Dr Jakub Šebesta
- The project focuses on extending spin-lattice dynamics simulations beyond cubic materials. The mentioned model represents a highly efficient scheme for describing magnetoelastic behaviour, such as magnetostriction and magnetoacoustic effects. The generalised model will provide the possibility to study and explain the magnetoelasticity of more complex compounds (alloys), paving the way towards materials with high application potential.

→ PROJECTS SUPPORTED BY THE TECHNOLOGY AGENCY OF THE CZECH REPUBLIC

M-ERA.NET Programme

FutureMold – Flexible manufacturing approach for recyclable bio-based high performance composite molds (2024–2026)

- Project ID: TQ05000004
- Principal Investigator: Dr Tomáš Brzobohatý
- The project focuses on the production of composite parts using a new concept of a recyclable, highly durable composite mold. The technologies developed within the project will significantly contribute to the European Green Deal programme, as the main goal is to substantially reduce CO_2 emissions in the production of composite material products.

IT4I

Program TREND

Optimization of design and production processes of vertical pumps using modern technologies (2024–2026)

- Project ID: FW10010202
- Principal Investigator: Doc. Tomáš Blejchař
- The aim of the project is to develop a modernised range of vertical pumps with improved hydraulic parameters, designed using know-how in hydraulic design (software) and new manufacturing processes (3D printing – WAAM welding technology). The R&D activities of the project will be validated on a model pump. The project focuses on a comprehensive upgrade of vertical pumps in line with current market requirements.

→ PROJECTS SUPPORTED BY THE MINISTRY OF INDUSTRY AND TRADE OF THE CZECH REPUBLIC

Operational Programme Technologies and Application for Competitiveness

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

- Project ID: CZ.01.01.01/01/22_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.

EyeERP – complex ERP system for eye clinics with mobile application MojeOči for performing and AI analysis of eye tests (2023–2026)

- Project ID: CZ.01.01.01/01/22_002/0000436
- Principal Investigator: Dr Tomáš Martinovič
- The aim of the project, supported by the Operational Programme Technology and Application for Competitiveness, is to create a comprehensive ERP system for eye clinics, together with a mobile application called MojeOči designed for AI-based analysis of eye tests. The project beneficiary is Apollo Data s.r.o.

Advanced medical data visualization with AI support (2024–2026)

- Project ID: CZ.01.01.01/01/22_002/0001028
- Principal Investigator: Dr Petr Strakoš
- The project, carried out in collaboration with the Misterine company, will use artificial intelligence methods to automatically detect various structures in tissues, such as blood vessels, healthy tissue, tumours, etc. The reason is that currently available imaging methods, such as MRI or CT, only provide a basic visualisation of results, and it is up to the specialist to interpret what they see based on black-and-white images. The project also aims to develop visualisation tools for presenting the results in virtual reality.

→ PROJECT SUPPORTED BY THE MINISTRY OF THE INTERIOR OF THE CZECH REPUBLIC

Research on holistic model of interconnected critical electricity and communication infrastructures (2023–2025)

- Project ID: VK01030109
- Principal Investigator: Dr Pavel Praks
- The project brings together three research centres (CVOOZE, SIX, and IT4Innovations) and creates an interdisciplinary Principal Investigator team with available expertise focused on examining the interconnections between individual critical infrastructures (control, data, and energy). The aim is to strengthen their resilience, robustness, and preparedness against potential risks, threats, or domino effects.

VSB-TUO Projects with IT4Innovations Participation

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

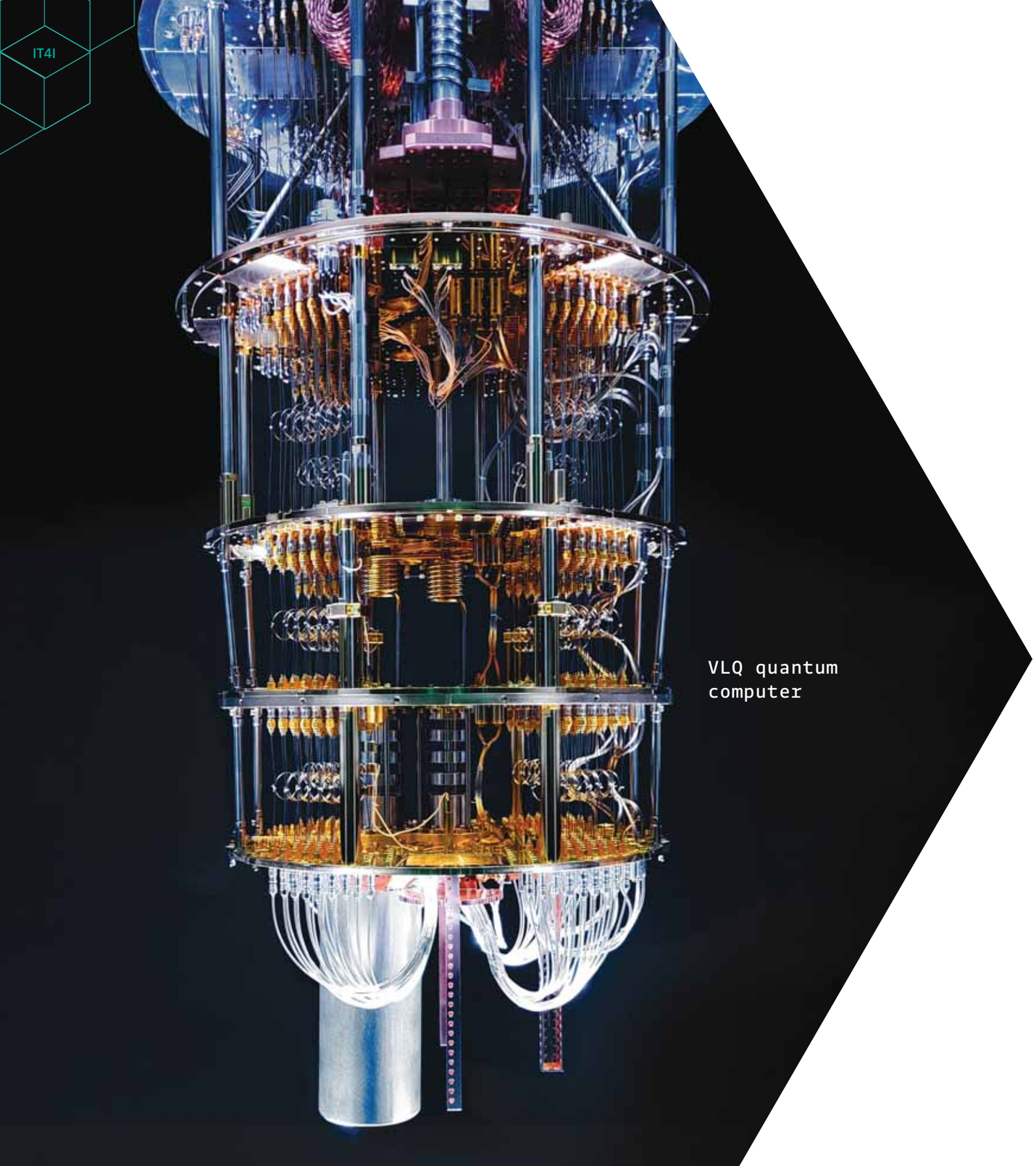
- Project ID: CZ.10.03.01/00/22_003/0000048
- IT4Innovations Coordinator: Prof. Tomáš Kozubek
- Grant Provider: Ministry of the Environment (State Environmental Fund of the Czech Republic), Operational Programme Just Transition 2021–2027
- The REFRESH project is a key tool for implementing the SMARAGD 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.

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 (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.

Center of Energy and Environmental Technologies (2020–2024)

- Project ID: TK03020027
- IT4Innovations Coordinator: Dr Pavel Praks
- Grant Provider: Technology Agency of the Czech Republic, THÉTA Programme
- The main aim of the project was to develop a modular, mobile, robust, and scalable technological solution for the efficient conversion of alternative fuels, waste, and by-products (used as alternative raw materials) into usable chemicals and valuable forms of energy, their storage, and efficient utilisation. This was supported by state-of-the-art methods, BIM, and digital twin technologies, in line with the principles of the circular economy.



VLQ quantum computer

Combination of Holographic and Digital Safety P rotection (2023–2025)

- Project ID: FW06010089
- Principal Investigator: Doc. Kamil Postava
- Grant Provider: Technology Agency of the Czech Republic, TREND Programme
- 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.

National Centre for Energy II (2023–2028)

- Project ID: TN02000025
- IT4INnovations Coordinator: Dr Pavel Praks
- Grant Provider: Technology Agency of the Czech Republic, National Centres of Competence Programme
- The mission of the National Centre for Energy II is to stimulate long-term cooperation between leading research organisations and key market players in the energy sector. Through applied research and the development of new methods, materials, and technologies, it focuses on increasing the efficiency, safety, and reliability of existing energy units, improving the reliability and security of energy networks, effectively deploying and operating decentralised energy sources, and utilising alternative fuels to ensure raw material independence and energy self-sufficiency for the Czech Republic. The goal is to create a comprehensive strategy for a modern, low-carbon, and sustainable energy sector, in line with strategic documents at both national and international levels.

09
INTERNATIONAL PROJECTS

Research and Development Projects

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

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

- Project ID: 956137 (H2020-JTI-EuroHPC-2019-1, EuroHPC-IA)
- Principal Investigator: Dr Jan Martinovič
- The project aimed 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 high-end supercomputers of that time and the exascale supercomputers of the future, thus fostering European competitiveness in this field. The proposed fully integrated LIGATE solution enabled the delivery of drug design campaign results with the highest speed and accuracy, as well as autotuning of the solution parameters to meet time and resource constraints.
- www.ligateproject.eu

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

- Project ID: 957269 (H2020-ICT-2018-20 / H2020-ICT-2020-1)
- Principal Investigator: Dr Kateřina Slaninová
- The project developed a holistic approach for co-designing computation and communication in a high-tech and particularly secure system for High-Performance Data Analysis. This was 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 validated 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

ACROSS – HPC big dAta artifiCial intelligence cross stack platfoRm tOwardS exaScale (2021–2024)

- Project ID: 955648 (H2020-JTI-EuroHPC-2019-1, EuroHPC-IA)
- Principal Investigator: Dr Jan Martinovič
- The project proposed and developed 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 leveraged 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 combined traditional HPC techniques with AI (specifically machine learning/deep learning) and BD analytic techniques to enhance the application test case outcomes.
- **www.acrossproject.eu**

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

- Project ID: 955811 (H2020-JTI-EuroHPC-2019-1, EuroHPC-RIA)
- Principal Investigator: Dr Jan Martinovič
- The project aimed 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 efficiently used storage tiers spanning NVMe and NVRAM at the top and tape-based technologies all the way down. Advanced I/O instrumentation and monitoring features were developed within the project, leveraging the latest AI and machine learning advancements to systematically analyse telemetry records and make smart decisions on data placement.
- **www.iosea-project.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 Innovation 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 aimed to push the current boundaries of a predictive understanding of biodiversity dynamics by developing a Digital Twin that provided advanced modelling, simulation, and prediction capabilities. By exploiting existing technologies and data available across relevant research infrastructures in new ways, the project enabled the interaction between species and their environment to be modelled accurately. Thus, scientists used BioDT to better observe biodiversity changes, 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 brought together a dynamic team of experts in biodiversity, High-Performance Computing, and Artificial Intelligence.
- www.biodt.eu

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

- Project ID: 101070014 (HORIZON-CL4-2021-HUMAN-01, RIA)
- Principal Investigator: Dr Jan Martinovič
- In the 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.
- www.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.
- www.dto-bioflow.eu

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KAR0L1NA

The Karolina supercomputer

FALCON – Foreseeing the next generation of Aircraft: hybrid approach using Lattice-Boltzmann, experiments and modelling to optimize fluid/struC-ture interactiONs (2024–2027)

- Project ID: 101138305 (HORIZON-CL5-2023-D5-01-09)
- Principal Investigator: Doc. Lubomír Říha
- Aviation transport is the second biggest source of greenhouse gas emissions after road transport. One of the main levers to decrease CO_2 emissions is to reduce the airframe structural weight. The growing amount of air traffic means that many EU citizens are still exposed to high noise levels. FALCON's ambition is to enhance the design capabilities of the European aircraft sector, focusing on fluid-structure interaction (FSI) phenomena to improve the aerodynamic performances of aircraft. Specifically, FALCON aims to develop high-performance, predictive, and multi-disciplinary tools for FSI in aeronautics in order to reduce the aeroacoustics and aeroelastic instabilities using multi-fidelity optimisation.
- falconproject.eu

POP3 – Performance Optimisation and Productivity 3 (2024–2026)

- Project ID: 101143931 (HORIZON-EUROHPC-JU-2023-COE-01)
- Principal Investigator: Doc. Lubomír Říha
- The Centre of Excellence for Performance Optimisation and Productivity (POP CoE) was established in October 2015 with the primary goal of assisting the broad community of HPC application developers and users in both scientific and industrial fields. Its aim is to help them understand performance-related issues in their applications and thereby improve their efficiency and productivity. The current project, entitled Performance Optimisation and Productivity 3 (POP3), is divided into three main pillars: services, users, and code design. The services provided within the POP project focus primarily on performance assessments, aiming to evaluate code performance and scalability, identify the main sources of inefficiency, and provide insights and recommendations on how to improve it.
- www.pop-coe.eu

AVITHRAPID – Antiviral Therapeutics for Rapid Response Against Pandemic Infectious Diseases (2024–2028)

- Project ID: 101137192 (HORIZON-HLTH-2023-DISEASE-03, RIA)
- Principal Investigator: Dr Jan Martinovič
- The project aims to support the search for new broad-spectrum antiviral compounds by developing various methods. Based on an existing set of small bioactive molecules, AVITHRAPID seeks to develop preclinical candidates targeting several viruses. This will be achieved by combining relevant expertise in preclinical drug discovery, including molecular modelling, biochemical and cellular assays, X-ray crystallography, medicinal chemistry, biophysical binding studies, ADMETox profiling, in vitro and in vivo pharmacokinetics, as well as animal disease models.
- www.avithrapid.eu

CLARA – Center for Artificial Intelligence and Quantum Computing in System Brain Research (2024–2030)

- Project ID: 101136607 (HORIZON-WIDERA-2023-ACCESS-01-01-two-stage, CSA)
- Principal Investigator: Doc. Vít Vondrák
- The Center for Artificial Intelligence and Quantum Computing in System Brain Research (CLARA) is an interdisciplinary Centre of Excellence focused on a new generation of artificial intelligence/machine learning applications and quantum-oriented supercomputing tools that will push the boundaries of research into neurodegenerative diseases, especially Alzheimer's disease. Within the project, a domain-specific platform for a hybrid computing and data infrastructure will be developed, based on emerging computing resources from the EuroHPC Joint Undertaking. This platform will significantly contribute to the development of the European computing and data ecosystem in the field of systematic brain research.
- www.clara-center.eu

EOSC-ENTRUST: A European Network of TRUSTed research environments (2024–2027)

- Project ID: 101131056 (HORIZON-INFRA-2023-EOSC-01, RIA)
- Principal Investigator: Doc. Vít Vondrák
- The mission of the project is to create a European network of trusted research environments for sensitive data and to support Europe's interoperability by establishing a common framework for federated data access and analysis. Within the project, four flagship cases were selected, focusing on genomics, clinical studies, social sciences, and public-private partnerships. These serve to compare capabilities, provide input for the design of the framework, and demonstrate secure data analysis using federated workflows.
- www.eosc-entrust.eu

TWIN SYNERGIES – Empowering participation and accelerating synergies in Widening countries with a focus on Green & Digital Transition (2024–2026)

- Project ID: 101160135 (HORIZON-WIDERA-2023-ACCESS-04)
- Principal Investigator: Martin Duda
- The project is focused on supporting the EU's strategic context regarding the creation of synergies at the operational and management levels and aims at so-called upstream synergies – the development of human resources and internationalisation. In this way, particular attention will be given to smart specialisation strategies, which are essential tools for creating combined effects with the smart growth strategy instruments at the EU level (especially with the Horizon Europe programme). The TWIN SYNERGIES project, which brings together 9 partners from 4 so-called Widening countries and 1 EU Member State, will, over its 24-month duration, develop and implement compatible, tailored, yet transferable activities for capacity building, internationalisation, human resource development, cooperation, valorisation, and technology deployment, with a focus on current developments related to the green and digital transition.
- www.twinsynergies.net

Digital Europe Programme

EUROCC 2 – 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 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 the 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.

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

EPICURE – High-level specialised application support service in High-Performance Computing (HPC) (2024–2028)

- Project ID: 101139786 (DIGITAL-EUROHPC-JU-2022-APPSUPPORT-01)
- Principal Investigator: Doc. Lubomír Říha
- The aim of the EPICURE project is to operate an HPC application support service for European scientists and researchers using EuroHPC JU supercomputers. The application support teams provide services focused primarily on application deployment, optimisation, and the correct execution of key applications, as well as on organising training events and workshops within major international HPC events. A unified contact point will also be established, enabling HPC users to obtain information about the systems, their architecture, access mechanisms, and available support services.
- https://epicure-hpc.eu/

Educational Projects

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
- Principal Investigator: Karina Pešatová
- 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

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LIST OF ABBREVIATIONS

AI	Artificial Intelligence
AIOPEN	European Space Agency project
ACROSS	HPC big dAta artifiCial intelligence cross stack platfoRm tOwardS exaScale
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
CLARA	Centre for AI and Quantum Computing in Systematic Brain Research
DICE	Data Infrastructure Capacity for EOSC
DOI	Digital Object Identifier
DTO-BioFLOW	Integration of biodiversity monitoring data into the Digital Twin Ocean
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's Programme focused on High-Performance Computing
EUPEX	EUropean Pilot for EXascale
EUROCC	National Competence Centres for HPC within the EuroHPC JU network
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
FEM	Finite Element Method
FAIR data	Data managed in line with FAIR principles (Findable, Accessible, Interoperable, Reusable)
Flop/s	Floating Point Operations per Second
FTE	Full-Time Equivalent
GAČR	Czech Science Foundation
GPU	Graphics Processing Unit
H2020	Horizon 2020
HPC	High-Performance Computing
HPCSE	High Performance Computing in Science and Engineering conference
HPDA	High-Performance Data Analytics
ICT	Information and Communication Technologies
IF	Impact Factor (indicator reflecting 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-Q	Large Unified Modern Infrastructure for Quantum Computing
MaX	MAterials design at the eXascale, European Centre of Excellence
OP JAK	Operational Programme Johannes Amos Comenius
OP TAK	Operational Programme Technology and Application for Competitiveness
POP3	Performance Optimisation and Productivity 3, European Centre of Excellence
PRACE	Partnership for Advanced Computing in Europe
PRACE-6IP	6IP – PRACE 6th Implementation Phase
QC	Quantum Computing
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
TAČR	Technology Agency of the Czech Republic
VI-HPS	Virtual Institute – High Productivity Supercomputing
VLQ	Quantum computer procured under the LUMI-Q consortium, installed at IT4Innovations
VŠB-TUO	VSB – Technical University of Ostrava
WHPC	Women in High Performance Computing

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VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

Postal Address

VSB – Technical University of Ostrava
17. listopadu 2172/15
708 00 Ostrava
Czech Republic
E info@it4i.cz
T +420 597 329 500

Address

IT4Innovations National Supercomputing Center
Studentská 6231/1b
708 00 Ostrava
Czech Republic

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