

# RESEARCH AT IT4INNOVATIONS

Our supercomputers support European  
science, industry, and society



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

IT4Innovations currently operates three supercomputers – Barbora, NVIDIA DGX-2, a specialized system for AI calculations, and a petascale system called Karolina with a theoretical peak performance of about 15.7 PFlop/s.

Czech research communities also have access to the LUMI supercomputer, thanks to IT4Innovations' membership in the eponymous consortium. Located in the Finnish town of Kajaani, LUMI is the most powerful European supercomputer with a theoretical peak performance of 580+PFlop/s. IT4Innovations also participates in its operation.

## RESEARCH LABS



**1. The Advanced Data Analysis and Simulations Lab** specialises in advanced data analysis, research and development in HPC co-design, data analysis and cloud technologies to enhance industry and society, programming models for HPDA, artificial intelligence, modelling, simulation, and application of dynamical systems.

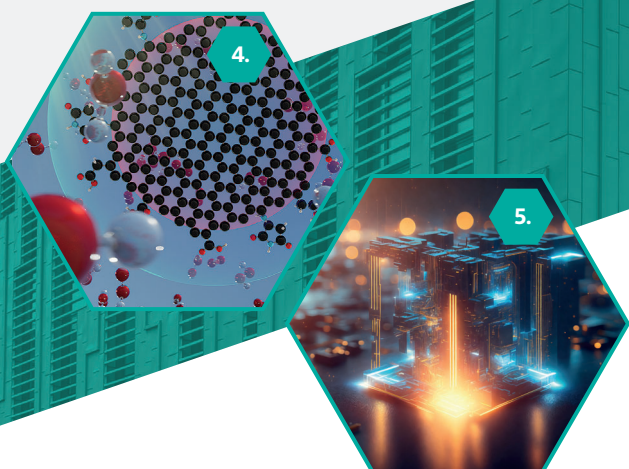
**2. The Infrastructure Research Lab** focuses on developing and accelerating parallel applications, code analysis, performance and scalability optimisation, as well as HPC application energy-efficiency optimisation, development of services provided to the infrastructure users, medical data processing, scientific data visualisation, and virtual and augmented reality.

**3. The Parallel Algorithms Research Lab** is primarily targeted on providing support for industry. The research team conducts applied research in developing scalable algorithms and HPC lib-

raries, numerical modelling and simulations, and the deployment of artificial intelligence in engineering.

**4. Modelling for Nanotechnologies Lab** is engaged in design, computer modelling, and preparation and experimental characterisation in the field of advanced nanomaterials and nanotechnology. It is also dedicated to developing special surfaces for nano-optics and has state-of-the-art experimental equipment for studying nano-systems.

**5. Quantum Computing Lab** is dedicated to developing new algorithms for quantum computers and simulators, including their practical applications, quantum error correction, research in quantum technologies, communication, cryptography, optimization and machine learning.



## CERTIFICATION

- ISO 9001 Quality Management System
- ISO 27001 Information Security Management System

## THE NATIONAL COMPETENCE CENTRE IN HPC

The reference and the single point of contact and coordination in Czechia for high-performance computing (HPC) and data analysis (HPDA).

[www.eurocc-czechia.cz/en](http://www.eurocc-czechia.cz/en)

## EUROPEAN DIGITAL INNOVATION HUB OSTRAVA

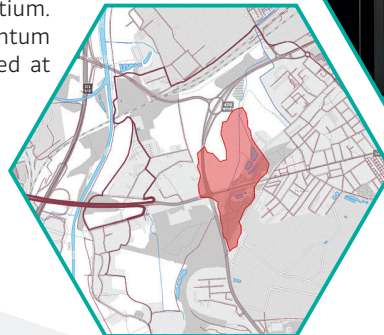
Supports the deployment and use of digital technologies primarily in small and medium-sized companies.

[www.edihostrava.cz/en](http://www.edihostrava.cz/en)



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

In 2023, IT4Innovations signed a hosting agreement with the EuroHPC JU as leader of the LUMI-Q consortium. Under this agreement, one of the six EuroHPC quantum computers in Europe will be installed and operated at IT4Innovations.



## SUPERCOMPUTERS

	NVIDIA DGX-2	Barbora	Karolina	LUMI
Put into operation	Spring 2019	Autumn 2019	Summer 2021	Autumn 2022
Theoretical peak performance	130 TFlop/s	849 TFlop/s	15,7 PFlop/s	580+ PFlop/s
Compute nodes	1	201	831	5,042
Accelerators in total	16x NVIDIA Tesla V100	32x NVIDIA Tesla V100	576x NVIDIA Tesla A100 2x NVIDIA RTX 6000	11,912x AMD Instinct MI250X 8x NVIDIA A40 GPU
CPU cores in total	48	7,232	106,880	454,784

[www.it4i.eu](http://www.it4i.eu)

### IT4INNOVATIONS IS A PROUD MEMBER OF:

- BDVA (Big Data Value Association)
- EUDAT CDI (EUDAT Collaborative Data Infrastructure)
- EuroHPC Joint Undertaking
- ETP4HPC (European Technology Platform in the area of High-Performance Computing)
- PRACE (Partnership for Research and Advanced Computing in Europe)
- EOSC (European Open Science Cloud)
- LUMI (Large Unified Modern Infrastructure)
- iRODS (Integrated Rule-Oriented Data System)

### EDUCATION AND TRAINING ACTIVITIES

- 25 courses, workshops, conferences a year
- EUMaster4HPC



# SELECTED PROJECTS

## **AVITHRAPID (Antiviral Therapeutics for Rapid Response Against Pandemic Infectious Diseases)**

AVITHRAPID aims to support the search for novel broad-spectrum antiviral compounds by advancing multiple approaches. Within the project, an early-stage drug discovery pipeline will be established that can be used to identify and develop novel antiviral compounds against emerging diseases rapidly.

## **BioDT (Biodiversity Digital Twin for Advanced Modelling, Simulation and Prediction Capabilities) [www.biodt.eu](http://www.biodt.eu)**

BioDT aims to push the current boundaries of a predictive understanding of biodiversity dynamics by developing a Digital Twin providing advanced modelling, simulation, and prediction capabilities. By exploiting existing technologies and data available across relevant research infrastructures in new ways, the BioDT project will be able to accurately model the interaction between species and their environment.

## **DTO-BioFlow (Integration of biodiversity monitoring data into the Digital Twin Ocean) [dto-bioflow.eu](http://dto-bioflow.eu)**

The project aims to provide innovative and sustainable solutions for making previously unavailable or hard-to-access biodiversity data accessible. It will pilot cost-effective and scalable technologies for monitoring species on a large scale.

## **EPICURE (High-level specialized application support service in High-Performance Computing)**

Application Support Teams will provide services aimed at application porting, optimisation and execution of key applications and organisation of specialised training events and workshops in the context of high-profile international HPC events. Finally, developing a single point of contact will allow European HPC users to retrieve information on the systems, their architectures, access mechanisms, and available support services.

## **EUPEX (European Pilot for Exascale) [www.eupeex.eu](http://www.eupeex.eu)**

The EUPEX consortium aims to design, build, and validate the first EU platform for HPC, covering end-to-end the spectrum of required technologies with European assets, from the architecture, processor, system software, and development tools to the applications. Scientifically, EUPEX is a vehicle to prepare HPC, AI, and Big Data processing communities for upcoming European Exascale systems and technologies.

## **EUROCC2 (National Competence Centres in the Framework of EuroHPC) [www.eurocc-czechia.cz/en](http://www.eurocc-czechia.cz/en)**

The mission of the National Competence Centre in HPC (NCC) is to offer a broad portfolio of services. It currently offers courses, webinars, or workshops in relevant areas. The services also include consulting, designing, and implementing pilot HPC solutions or migrating existing ones. In addition, it also facilitates partnerships between academia, government, and the private sector.

## **EXA4MIND (EXtreme Analytics for MINing Data) [www.exa4mind.eu](http://www.exa4mind.eu)**

The EXA4MIND project will build an Extreme Data platform that brings together data storage systems and powerful computing infrastructures by implementing novel automated data management and effective data

staging. Four application cases from molecular dynamics drive the project: advanced driver assistance systems, smart agri-viticulture, and health and social Big Data.

## **FALCON (Foreseeing the next generation of Aircraft: hybrid approach using Lattice-Boltzmann, experiments and modelling to optimize fluid/structure interactions)**

The project aims to increase the competitiveness of the European aerospace industry by focusing on the development of Fluid-Structure Interaction (FSI) phenomena to improve the aerodynamic performance of aircraft. Specifically, the project aims to develop high-performance, predictive and multidisciplinary tools for FSI in aeronautics to reduce the aeroacoustics and aeroelastic instabilities using multi-fidelity optimisation.

## **MAX (MAterials design at the eXascale) [www.max-centre.eu](http://www.max-centre.eu)**

Materials simulations have become one of the most intensive and fast-growing domains for high-performance computing worldwide. The MAX project will target these lighthouse 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 both scientific and industrial applications.

## **OpenWebSearch.EU (Piloting a Cooperative Open Web Search Infrastructure to Support Europe's Digital Sovereignty) [www.openwebsearch.eu](http://www.openwebsearch.eu)**

The project consortium aims to develop an open European infrastructure for web search. Within three years, the researchers will develop the core of a European Open Web Index as a basis for a new Internet Search in Europe. In addition, the project will set the foundation for an open and extensible European Open Web Search and Analysis Infrastructure based on Europe's values, principles, legislation, and standards.

## **POP3 (Performance Optimisation and Productivity 3) [www.pop-coe.eu](http://www.pop-coe.eu)**

POP services mainly focus on performance assessments to evaluate code performance and scale, identifying the main sources of inefficiency or improving energy efficiency. POP3 will focus on the European flagship HPC applications for other CoEs and will still provide services to prescribers and SMEs to promote the efficient use of computing resources.

## **SPACE (Scalable Parallel and distributed Astro-physical Codes for Exascale) [www.space-coe.eu](http://www.space-coe.eu)**

In Astrophysics and Cosmology, High-Performance Computing-based numerical simulations are outstanding instruments for scientific discovery. The SPACE Centre of Excellence aims to extensively re-engineer target codes to engage with new computational solutions and adopt innovative programming paradigms, software solutions, and HPC libraries.