Review 2021

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

Our supercomputers support science, industry, and society.

Table of Contents

Managing Director's Introduction

Dear readers and supporters of IT4Innovations National Supercomputing Center,

Here we are with the latest release of the publication that summarises the activities of our supercomputing centre over the past year. This year was certainly special for our institute and our supercomputing centre, which celebrated ten years since its establishment. Although the plans for grand celebrations with the presence of prominent personalities were thwarted by the coronavirus crisis, we managed to celebrate the event at least among the IT4Innovations staff. Such an anniversary also calls for renewed graphic design of this publication, which I hope you will enjoy for its clarity and originality.

The biggest and most watched event of last year, however, was the commissioning of the Karolina supercomputer. The Czech Republic's most powerful supercomputer, which was acquired as part of the pan-European EuroHPC Joint Undertaking, has been available to our users since August 2021. With its peak performance of 15.7 PFlop/s, it was ranked among the top 100 most powerful supercomputers in the world after its launch, and according to the GREEN500 it is even the eighth most energy-efficient supercomputer in the world!

Thanks to our involvement in the LUMI consortium, our users could for the first time also compute on the LUMI supercomputer, namely on its non-accelerated part. The LUMI-C pilot call resulting in two Czech projects being selected kicked off an era in which Czech researchers will be able to use the computational resources of one of the world's most powerful supercomputing systems with a performance of more than half an exaflop per second. IT4Innovations also participates at the very building of the LUMI supercomputer and its operation.

Though we were pleased to introduce two new supercomputers to our users - the Karolina and LUMI supercomputers, we also had to say goodbye to two of our long-time members in 2021. The Anselm supercomputer went to silicon heaven after seven years of operation. The first ever supercomputer in IT4Innovations has moved to the Ostrava World of Technology, where thousands of visitors admire it as part of the exhibition. In December, the Salomon supercomputer also performed its last task. The 40th most powerful supercomputer of its time performed 8,700,000 computational tasks over 1,085 research projects.

We have continued to provide computational resources to the scientific community and industry; in total, 328 projects were supported with more than 280 million core hours allocated. Among the projects carried out on our supercomputers, I would like to highlight a project in which scientists from several Czech research institutes, including IT4Innovations, were the first in the world to observe inhomogeneous electron charge distribution on an atom, thus confirming a 30-year-old theoretical prediction. The breakthrough discovery was published in the prestigious Science journal.

I am also very pleased with our active role in international research activities. For example, our success in participating in projects within the European Union's Horizon 2020 framework programme for research and innovation is unique. Last year, IT4Innovations was involved in 16 international projects, one of which, LEXIS, was coordinated by us. The excellent research of IT4Innovations was also confirmed by the results of the European Innovation Radar, where we ranked among the key innovators of the Czech Republic with a total of seven innovations being supported by European projects.

Our cooperation with industrial companies is also promising, and we are continuously expanding it. Since 2020, we have been part of the Digital Innovation Hub, through which we help companies from the Moravian-Silesian Region to address their needs in the field of digitalisation. Last year, for example, we were behind the development of an intelligent weeding machine, cutting-edge virtual reality glasses used by car manufacturers, as well as a project aimed at making retinal screening more efficient by training neural networks.

Finally, I would like to thank all of our staff and partners who have worked together to meet our strategic goals and commitments, ensure the operation of our centre, and contribute to its further development despite the ongoing COVID-19 pandemic. I wish my colleagues, and all of you, all the best in the period ahead.

Vít Vondrák

Managing Director

↔ The IT4Innovations building was officially opened in 2014.

1

IT4Innovations Profile

IT4Innovations National Supercomputing Center at VSB – Technical University of Ostrava (VSB-TUO) is a leading research, development, and innovation centre active in the fields of High-Performance Computing (HPC), Data Analysis (HPDA), and Artificial Intelligence (AI) and their application to other scientific fields, industry, and society, and it operates the most powerful supercomputing systems in the Czech Republic. Together with the CESNET and CERIT-SC institutions, IT4Innovations constitutes **e-INFRA CZ**, a strategic research infrastructure of the Czech Republic. This infrastructure is listed on the National Roadmap for Large Infrastructures for Research, Experimental Development and Innovations, prepared by the Ministry of Education, Youth and Sports of the Czech Republic.

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

In 2021, IT4Innovations operated four supercomputers:

→ Salomon – 2 PFlop/s – in operation from summer 2015 to December 2021,
→ Barbora – 849 TFlop/s, installed in the autumn of 2019,
→ The specialised NVIDIA DGX-2 system for artificial intelligence computation – 130 TFlop/s and 2 PFlop/s in AI, installed in the spring of 2019,
→ Karolina – 15.7 PFlop/s, installed in the summer of 2021.

Apart from the supercomputers operated at IT4Innovations, Czech research communities also have access to the LUMI supercomputer, which is being installed in Kajaani, Finland. Thanks to IT4Innovations' membership in the LUMI consortium of ten European countries, Czech scientists will be able to use one of the world's most powerful and advanced supercomputers, with a theoretical peak performance which is expected to exceed 550 PFlop/s in 2022. IT4Innovations also participates at the very building of the LUMI supercomputer and its operation.

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

IT4Innovations' research activities are executed across five laboratories:

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

IT4Innovations also has a strong focus on cooperation with industrial enterprise, thanks to which IT4Innovations has been registered at the European Commission level as a Digital Innovation Hub (DIH), and has become a member of the European DIHnet EU network of digital innovation hubs. In this context, VSB – Technical University of Ostrava has developed a partnership with the Moravian-Silesian Innovation Centre Ostrava in order to co-found the Digital Innovation Hub Ostrava in 2020.

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

In 2021, IT4Innovations became a member of the international project EUMaster4HPC consortium that is implementing the first pan-European Master's degree programme focused purely on HPC, with its launch being scheduled for the 2022 winter semester.

History

• **2011** → The foundation of IT4Innovations → Membership in PRACE (Partnership for Advanced Computing in Europe) • **2013** → Launching of the Anselm supercomputer • **2014** → Opening of the IT4Innovations building • **2015** → Launching of the Salomon supercomputer • **2016** → Membership in ETP4HPC (European Technology Platform for High-Performance Computing) • **2018** → The Czech Republic joins the EuroHPC JU, in which IT4Innovations is actively involved → IT4Innovations becomes part of the H2020 POP2 Centre of Excellence and is registered by the European Commission as a DIH • **2019** → Launching of the Barbora supercomputer and the NVIDIA DGX-2 → Membership in BDVA (Big Data Value Association) and EUDAT CDI (EUDAT Collaborative Data Infrastructure) → Foundation of e-INFRA CZ → Launching of the H2020 LEXIS project, the coordinator of which is IT4Innovations • **2020** → Foundation of the Digital Innovation Hub Ostrava → IT4Innovations becomes the National Competence Centre in HPC • **2021** → Launching of the Karolina supercomputer → Termination of operation of the Anselm and Salomon supercomputers → Membership in EOSC Association

Mission, Vision, Values, and Memberships

Mission

Our mission is to carry out excellent research in the field of high-performance computing and advanced data analysis, and to operate the leading national supercomputing infrastructure in the Czech Republic, strengthening 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 the field of high-performance computing and processing of advanced data sets for the benefit of science, industry, and the whole of society.

IT4Innovations values

Professionalism · Innovativeness · Team work · IT4Innovations brand

Memberships

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

→ BDVA/DAIRO – Big Data Value Association/Data, AI and Robotics
→ EOSC – European Open Science Cloud
→ ETP4HPC – European Technology Platform for High-Performance Computing
→ EUDAT CDI – EUDAT Collaborative Data Infrastructure
→ I4MS – ICT Innovation for Manufacturing SMEs
→ LUMI – Large Unified Modern Infrastructure
→ PRACE – Partnership for Advanced Computing in Europe

Organisational Structure

Organisational Structure of IT4Innovations

Scientific Council | Managing Director | Doc. Vít Vondrák

- Research and Development Department | Prof. Tomáš Kozubek
  - Advanced Data Analysis and Simulations Lab | Dr Jan Martinovič
  - Infrastructure Research Lab | Dr Lubomír Říha
  - Parallel Algorithms Research Lab | Dr Tomáš Karásek
  - Modelling for Nanotechnologies Lab | Prof. Michal Otyepka
  - Big Data Analysis Lab | Prof. Miroslav Vozňák
  - Training and Education Office | Karina Pešatová
- Supercomputing Services Department | Dr Branislav Jansík
  - HPC Operations and Administrations Department | Radovan Pasek
  - User Support Department | Petra Lyčková Navrátilová
- Communications Department | Zuzana Červenková
- Public Procurement and Legal Services Department | Jan Juřena
- Finance Department | Petr Válek
- Administrations and Operations Department | Helena Starková
- Development Department | Martin Duda

Scientific Council of IT4Innovations

Chairman | Doc. Vít Vondrák

Members Internal

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

Members External

- Prof. Jiří Damborský | Loschmidt laboratories of Masaryk University Brno
- Doc. Jiří Jaroš | Faculty of Information Technology, Brno University of Technology
- Dr Jakub Šístek | Mathematical Institute 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 2021, the number of employees of IT4Innovations by divisions (in full time equivalent, FTE) was 148.55 FTE in total, which consists of:

21% Management and Administration

14% Supercomputing Services

65% Research and Development

- 42% Advanced Data Analysis and Simulations Lab
- 14% Infrastructure Research Lab
- 23% Parallel Algorithms Research Lab
- 16% Modelling for Nanotechnologies Lab
- 5% Big Data Analysis Lab

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

2

Important Events in 2021

JANUARY

The Ministry of Industry and Trade (MIT) announces the winners of the national call for European Digital Innovation Hubs. These will support the digitalisation of SMEs and public administration authorities. One of the winners is the **Digital Innovation Hub Ostrava**.

We cooperate with the ENET Centre, which is part of VSB – Technical University of Ostrava, in the **Centre for Energy and Environmental Technologies** (CEET) project.

IT4Innovations joins the **SCALABLE** (SCAlable LAttice Boltzmann Leaps to Exascale) project, which supports the development of European exascale systems and will support fundamental research through advanced computational fluid dynamics methods.

IT4Innovations becomes part of the **DICE** (Data Infrastructure Capacity for EOSC) project, which links a network of computing and data centres, research infrastructures, and data repositories to create a European Open Science Cloud (EOSC) infrastructure for data management and storage.

IT4Innovations joins the **LIGATE** (LIgand Generator and portable drug discovery platform AT Exascale) project, where European supercomputing systems will be used to improve computer-aided drug design.

FEBRUARY

The first ever Ostrava supercomputer, Anselm, leaves IT4Innovations. It finds a new home at the Science and Technology Centre in Ostrava's Dolní Vítkovice area.

MARCH

IT4Innovations develops a simulation that helps set up a large-scale vaccination centre in Ostrava.

IT4Innovations becomes part of the ACROSS (HPC big dAta artifiCial intelligence cross stack platfoRm tOwardS exaScale) project, which will develop a platform combining HPC, Big Data, and AI. This will support applications in the fields of aviation, climate, weather, and energy.

The PROJECT large-capacity data storage facility is put into operation to store and back up data processed or generated on the Ostrava supercomputers.

APRIL

The IO-SEA (IO Software for Exascale Architecture) project, of which IT4Innovations is a part, kicks off. The aim of the project is to develop a data management and storage platform using the latest advances in artificial intelligence and machine learning to plan and optimise data transfers.

The excellent research of IT4Innovations is recognised by the Innovation Radar result, ranking IT4Innovations as one of the key innovators in the Czech Republic, with seven innovations supported by European projects.

MAY

The 24th May marks the 10th anniversary of the foundation of IT4Innovations.

JUNE

The Minho Manifesto declaration is signed, aiming to strengthen research related to high-performance computing and to link the five supercomputing centres that now have petascale systems more closely. The emerging European network includes IT4Innovations and supercomputing centres in Portugal, Slovenia, Bulgaria, and Luxembourg.

In the TOP500 list, which tracks the world's most powerful supercomputers, the Karolina supercomputer ranks 69th worldwide and 19th in Europe. In terms of energy efficiency, which is monitored by the Green500 list, the Karolina supercomputer ranks 15th, and in the HPCG list it ranks 38th.

JULY

IT4Innovations hosts a debate about the green future of Europe chaired by Frans Timmermans, the Executive Vice-President of the European Commission.

The e-INFRA CZ consortium, of which IT4Innovations is a part, implements quantum key distribution. Communication secured by encryption through quantum key distribution (QKD) represents a new shift in communication security and addresses the risks associated with the advent of quantum computers.

AUGUST

After a series of tests, the Karolina supercomputer is made available to users of computing infrastructure.

SEPTEMBER

Martin Golasowski from IT4Innovations wins the bronze award in the Joseph Fourier Prize competition for his project focused on optimisation of urban transport using intelligent navigation service.

The e-INFRA CZ consortium achieves the highest ranking in the international evaluation of large research infrastructures of the Czech Republic, which is held under the auspices of the MEYS of the Czech Republic.

Georg Zitzlsberger obtains two NVIDIA Deep Learning Institute (DLI) instructor certificates for the following courses: Building Transformer-Based Natural Language Processing Applications and Fundamentals of Deep Learning.

NOVEMBER

Scientists from several Czech research institutions including IT4Innovations are the first in the world to observe inhomogeneous electron charge distribution on an atom, thus confirming a 30-year-old theoretical prediction. Their paper is published in the prestigious Science journal.

The 'Supercomputing in Science and Engineering 2019–2020' conference proceedings are published, presenting 21 selected projects that were conducted using Ostrava supercomputers within the 13th up to the 19th Open Access Grant Competition.

Evaluating supercomputers in terms of their energy efficiency, the Green500 list as of November 2021 ranks the Karolina supercomputer, after its GPU-accelerated part upgrade, 8th worldwide. In Europe, it ranks 3rd.

The 5th IT4Innovations Users Conference is held.

DECEMBER

The Salomon supercomputer completes its last task. The era of the 40th most powerful supercomputer at the time ends after six years of operation.

Jakub Homola from the Infrastructure Research Lab receives the Prof. Babuška Prize for outstanding work in computer science for the year 2021. The expert jury awarded this prize for his masters thesis, in which he used our supercomputers.

The LEXIS (Large-scale Execution for Industry & Society) project, coordinated by IT4Innovations, is completed. The aim of the project was to create an advanced engineering platform by using modern technologies such as high-performance computing, big data, and cloud.

↔ NVIDIA-DGX2

IT4Innovations' supercomputing infrastructure was expanded in the spring of 2019 with the addition of a dedicated NVIDIA DGX-2 computing system. The system is designed to solve the most demanding AI tasks, achieving a peak performance of 2 PFlop/s.

3

Financial Review

Operational and Capital Expenditures

The total expenditure of IT4Innovations amounted to CZK 497,097,000, 41% and 59% of which were operating (non-investment) costs and investment (capital) costs, respectively.

The largest part of the operating costs consisted of salary expenses, services (costs of electricity consumption, maintenance of the operated systems and supporting infrastructure, technical and system support, etc.) and project overheads.

Compared to 2020, there was a significant increase in investment costs, from CZK 19,918,000 (2020) to CZK 291,833,000 (2021). This increase is mainly due to the costs associated with the acquisition of the new EuroHPC petascale Karolina supercomputer.

Operational expenditures structure
CZK 205,264,000 in total | 41%

- 39.3% Personnel costs – research labs
- 13.8% Personnel costs – management, administration
- 9.5% Personnel costs – supercomputing services
- 15.4% Services
- 15.4% Project overheads
- 1.5% Membership fees to international organisations and consortia
- 1.5% International and domestic business trips (including those of invited speakers)
- 1.1% Small fixed assets
- 1.0% Scholarships
- 0.7% Consumables
- 0.6% Depreciation
- 0.2% Other costs

Capital expenditures structure
CZK 291,833,000 in total | 59%

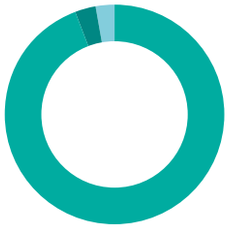
- 99.5% Tangible fixed assets – machines and equipment
- 0.3% Tangible fixed assets – buildings
- 0.2% Intangible fixed assets

Sources of Funding

In 2021 the overall budget of IT4Innovations was CZK 505,033,000. Investment costs accounted for 58% of total funding sources, while non-investment costs amounted to 42%. These funds include, among others, the difference between the creation and use of the specific purpose funds from previous years and the profit before tax. Structural Funds accounted for the largest share of funding sources, followed by national projects. The third most important source of funding for IT4Innovations was international projects. This was followed by: the long-term research organisation development fund, internal resources, contract research and rental of computational resources, and other sources.

Sources of funding – investment costs

CZK 291,833,000 in total



- 94.2% Structural funds (projects of the Operational Programme Research, Development and Education and projects of the Operational Programme Enterprise and Innovation for Competitiveness)
- 3.1% Internal resources
- 2.7% Long-term Research Organisation Development Fund

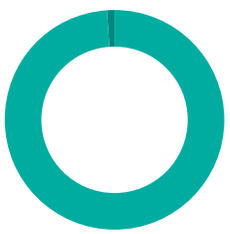
Sources of funding – non-investment costs

CZK 213,200,000 in total

- 38.7% National projects
- 26.9% International projects
- 12.2% Structural funds
- 9.2% Long-term Research Organisation Development fund
- 8.3% Internal resources
- 2.4% Contract research and rental of computational resources
- 2.3% Other

Structural funds

CZK 301,085,000 in total



- 99.1% Operational Programme Research, Development and Education – MEYS CR
- 0.9% Operational Programme Enterprise and Innovation for Competitiveness – MIT CR

National projects

CZK 82,478,000 in total

- 84.1% Large Infrastructures Projects for Research, Experimental Development, and Innovation – MEYS CR
- 6.3% TREND – TA CR
- 2.7% Standard projects – GA CR
- 2.3% Security research of the Czech Republic – Ministery of the Interior of the Czech Republic
- 2% Competence centres – TA CR
- 1.3% International grant projects evaluated on the LEAD Agency principle – GA CR
- 0.8% TRIO programme projects – MIT CR
- 0.3% Science and Research projects in the Moravian-Silesian Region – MSR
- 0.1% Researcher Mobility Support within international cooperation in R&D&I – MEYS CR
- 0.1% Individual projects – MSR

International projects

CZK 57,294,000 in total

- 40.6% EUROCC
- 18.9% LEXIS
- 7.1% POP2
- 6.7% PRACE 6IP
- 4.3% LIGATE
- 3.9% EVEREST
- 3.3% ACROSS
- 3.1% s-NEBULA
- 3% SCALABLE
- 2.9% IO-SEA
- 2.7% ExaQUte
- 2.2% OPENQKD
- 0.6% Cloudifacturing
- 0.4% TETRAMAX
- 0.3% SCtrain

List of IT4Innovations Projects

National Grants

Projects supported by the Ministry of Education, Youth and Sports

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

Projects of the Operational Programme Research, Development and Education
- IT4Innovations National Supercomputing Center – Path to Exascale
- e-INFRA CZ: Modernisation
- Doctoral School for Education in Mathematical Methods and Tools in HPC
- Technology for the Future 2.0
- Artificial Intelligence and Reasoning
- Science without Borders 2.0
- Modelling of Collision Processes in Low-Temperature Plasma
- Development of a tool for scientific data processing and visualisation in VR with multi-user support
- Novel sources of THz radiation based on spintronic effects
- Development of Computational Algorithms for Solution of Nonlinear Structural Dynamical Problems with Utilisation of ESPRESO Numerical Library

Researcher Mobility support within international cooperation in R&D&I
- Multiscale design of novel Rare Earth free permanent magnets

Projects supported by the Moravian-Silesian Region

Individual projects
- Digital Innovation Hub – Pilot Verification

Science and research project of the Moravian-Silesian Region
- Projects of talented VSB-TUO PhD students

Projects supported by the Grant Agency of the Czech Republic

International Grant Projects Evaluated by the Lead Agency
- Space-time Boundary Element Methods for the Heat Equation

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

Projects supported by the Technology Agency of the Czech Republic

National Centres of Competence Programme
- Personalised Medicine – Diagnostics and Therapy

TREND Programme
- Development of Expert System for Automatic Evaluation of Pathologies from Eye Images
- Research and development of a functional sample of a railway vehicle with the ability to collect data and software - a simulator with the ability to generate data for obstacle detection training in simulated conditions
- Creating a model for evaluating the impact of changes in the parameters of the tax-benefit system on the socio-economic situation of families with children in the Czech Republic

Projects supported by the Ministry of Industry and Trade

TRIO programme
- Intake and discharge objects of pump and turbine stations

Operational Programme Enterprise and Innovation for Competitiveness
- Digital twin of product within Siemens plants
- SmartFleet – AI based software for a full utilisation of electric cars in companies and maximisation of their share in the car fleet
- Holograms with active security elements

VSB-TUO Projects with IT4Innovations participation
- Employment of artificial intelligence into an emergency call Reception (project supported by the Ministry of the Interior of the Czech Republic)
- Optimisation of the electrical distribution system operating parameters using artificial intelligence (project supported by the Technology Agency of the Czech Republic)
- Contactless detector for partial discharges activity in medium overhead voltage powerlines (project supported by the Technology Agency of the Czech Republic)
- National Centre for Energy (project supported by the Technology Agency of the Czech Republic)
- Energy System for Grids (project supported by the Technology Agency of the Czech Republic)
- CEET – Centre for Energy and Environmental Technologies (project supported by the Technology Agency of the Czech Republic)

International grants

Projects of the 8th Framework Programme for Research and Innovations of the European Union — Horizon 2020
- EUROCC – National Competence Centres in the framework of EuroHPC
- LEXIS – Large-scale EXecution for Industry & Society
- POP2 – Performance Optimisation and Productivity 2
- PRACE-6IP – Partnership for Advanced Computing in Europe, 6th implementation phase
- LIGATE – LIgand Generator and portable drug discovery platform AT Exascale
- EVEREST – dEsign enVironmEnt foR Extreme-Scale big data analyTics on heterogeneous platforms
- ACROSS – HPC big dAta artifiCial intelligence cross stack platfoRm tOwardS exaScale
- s-NEBULA – Novel Spin-Based Building Blocks for Advanced TeraHertz Applications
- SCALABLE – SCAlable LAttice Boltzmann Leaps to Exascale
- IO-SEA – IO Software for Exascale Architecture
- ExaQUte – Exascale Quantifications of Uncertainties for Technology and Science Simulation
- OPENQKD – Open European Quantum Key Distribution Testbed
- CloudiFacturing – Cloudification of Production Engineering for Predictive Digital Manufacturing
- TETRAMAX – Technology Transfer via Multinational Application Experiments
- EXPERTISE – Experiments and High-Performance Computing for Turbine Mechanical Integrity and Structural Dynamics in Europe
- DICE – Data Infrastructure Capacity for EOSC

Erasmus+ projects
- SCtrain – Supercomputing knowledge partnership

4

Supercomputing Services

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

In 2021, IT4Innovations ran **four supercomputers**: **Salomon** (2 PFlop/s), **Barbora** (849 TFlop/s), the **NVIDIA DGX-2** system specialised in artificial intelligence calculations (130 TFlop/s and 2 PFlop/s in AI) and **Karolina** (15.7 PFlop/s).

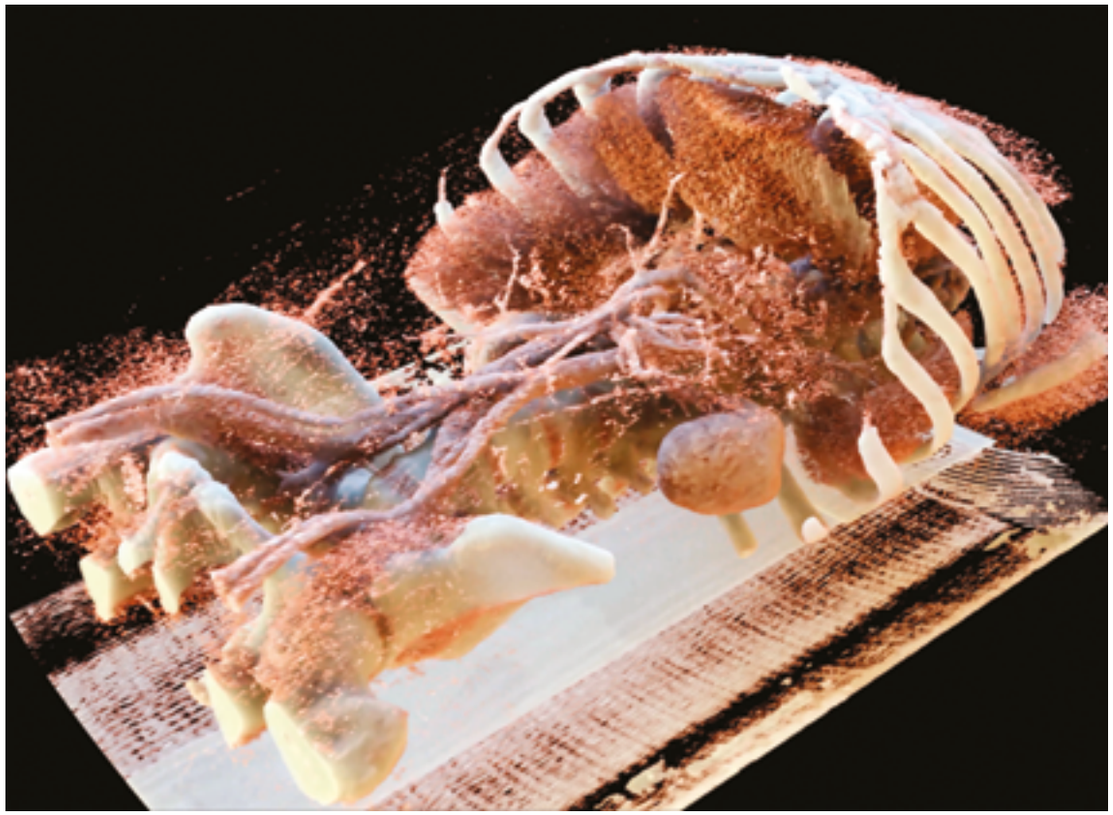
The **petascale Karolina system** was installed during the first half of the year and was fully operational by the summer of 2021. It was acquired as part of the pan-European EuroHPC Joint Undertaking, with 35% of its computational resources available to users from EuroHPC member nations. Immediately after its launch, it ranked among the most powerful HPC systems in Europe. In the TOP500 list, which evaluates supercomputers in terms of their performance, the Karolina supercomputer ranked 69th worldwide in 2021 and 19th in Europe. In the Green500 list of the most energy-efficient supercomputers it ranked 8th globally, which is third in Europe, and in the **HPCG list** it ranks 38th.

The fifth Ostrava supercomputer, supplied by Hewlett Packard Enterprise, was designed to comprehensively cover user requirements for solving complex scientific and industrial problems involving both classical numerical simulations and large-scale data analysis, potentially including the use of artificial intelligence.

At the beginning of the year, the operation of the very first Ostrava supercomputer, **Anselm**, was terminated. During its operation, it ran more than 2.6 million computational tasks over 725 research projects. Now the Anselm supercomputer is part of the Science and Technology Centre in Dolní Vítkovice area in Ostrava.

In 2021, work continued on the installation of one of the most powerful supercomputers in Europe and worldwide, the pre-exascale LUMI supercomputer, which will be commissioned during 2022 in Kajaani, Finland. Thanks to IT4Innovations' membership in the LUMI consortium, which consists of Finland as the Coordinator, as well as Belgium, the Czech Republic, Denmark, Estonia, Iceland, the Netherlands, Norway, Poland, Sweden, and Switzerland, scientific teams from the Czech Republic will also be able to perform computations on the LUMI supercomputer. IT4Innovations also participates at the very building of the LUMI supercomputer and its operation.

Another achievement in 2021 was the commissioning of the PROJECT large-capacity data storage facility. With a capacity of 15 petabytes, it is based on the latest technologies, specifically on the Spectrum Scale solution from IBM. The state-of-the-art solution promises ample capacity, reliable and fast operation, and will not only serve the specific data needs of existing supercomputers, but thanks to its modular architecture allowing subsequent updates and extension it will also offer its capacity to their successors.



↔ Medical data processing

In collaboration with medical doctors from the University Hospital Ostrava, IT4Innovations is developing tools for automatic segmentation and 3D reconstruction of tissue models from Computed Tomography (CT) and Magnetic Resonance Imaging (MRI) images.

Technical Specifications of the Supercomputers

	Salomon	NVIDIA DGX-2	Barbora	Karolina	LUMI-C
Put into operation	summer 2015	spring 2019	autumn 2019	summer 2021	autumn 2021
Theoretical peak performance	2 PFlop/s	130 TFlop/s, 2 Pflop/s for AI	849 TFlop/s	15.7 PFlop/s	6.3 PFlop/s
Operating system	CentOS 64bit 7.x	CentOS 64bit 7.x	CentOS 64bit 7.x	Centos 64 bit 7.x	Custom Cray
Compute nodes	1,008	1	201	831	1,536
CPU	2x Intel Haswell, 12 cores, 2.5 GHz, 24,192 cores in total	2x Intel Xeon Platinum, 24 cores, 48 cores in total	2x Intel Cascade Lake, 18 cores, 2.6 GHz, 7,236 cores in total	720x 2x AMD 7H12, 64 cores, 2.6 GHz, 92,160 cores in total 72x 2x AMD 7763, 64 cores, 2.45 GHz, 9,216 cores in total 72x 8x NVIDIA A100 GPU, 576 GPU in total 32x Intel Xeon-SC 8628, 24 cores, 2.9 GHz, 768 cores in total 36x 2x AMD 7H12, 64 cores, 2.6 GHz, 4,608 cores in total 2x 2x AMD 7452, 32 cores, 2.35 GHz, 128 cores in total	1376x AMD EPYC 7763, 2.45/3.5 GHz, 128 cores (2x64), 176,128 cores in total 128x AMD EPYC 7763, 2.45/3.5 GHz, 128 cores (2x64), 16,384 cores in total 32x AMD EPYC 7763, 2.45/3.5 GHz, 128 cores (2x64), 8,192 cores in total
RAM per compute node	128 GB, 3.25 TB (UV node)	1.5 TB DDR4, 512 GB HBM2 (16 x 32 GB)	192 GB 6 TB fat node	256 GB / 1 TB (GPU) / 24 TB fat node 320 GB HBM2 (8 x 40 GB) GPU	256 GB / 512 GB / 1,024 GB
GPU accelerators	N/A	16x NVIDIA Tesla V100 32 GB HBM2	32x NVIDIA Tesla V100	576x NVIDIA A100	N/A
MIC accelerators	864x Intel Xeon Phi 7120P	N/A	N/A	N/A	N/A
Storage	500 TB / home (6 GB/s), 1,638 TB / scratch (30 GB/s)	30 TB NVMe	29 TB / home, 310 TB / scratch (28 GB/s)	30.6 TB / home (1.93 GB/s sequential write performance, 3.10 GB/s sequential read performance), 1,361 TB / scratch (NVMe, 730.9 GB/s sequential write performance, 1, 198.3 GB/s sequential read performance)	80 PB (/home + /project + /scratch) 240 GB/s
Interconnection	Infiniband FDR 56 Gb/s	Infiniband FDR 56 Gb/s	Infiniband HDR 200 Gb/s	Infiniband HDR 200 Gb/s	200 Gb/s Slingshot-11

↔ In 2021, IT4Innovations operated four supercomputers: Salomon, Barbora, NVIDIA-DGX2, and Karolina.

Computational Resources Allocations

Providing computational resources is one of the main missions of IT4Innovations. Supercomputers have been available to the Czech scientific community and industrial companies continuously since 2013, when the Anselm supercomputer was launched. Between then and the end of 2021, a total of 1,424,682,320 core hours have been used, distributed among 1,582 projects across a broad range of scientific fields including the design of new materials and drugs, the discovery of physical laws, engineering problems, rendering and visualisation of scientific data, projects addressing cyber security, advanced data analytics, and others.

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

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

→ The largest share of the computational resources are distributed within the framework of Open Access Grant Competitions, which IT4Innovations announces three times a year. They are open to researchers and academics from the Czech Republic. Submitted projects are subject to the approval of the allocation committee based on an expert evaluation in terms of scientific excellence, computational readiness, and socio-economic impact.

→ Director's discretion – applications are submitted continuously, and only in cases where Open Access Grant Competitions cannot be used. This is an irregular allocation of computational resources approved by IT4Innovations management.

→ Rental of computational resources – This is paid access to the computational resources of the supercomputers operated, which is charged at market rates according to the current IT4Innovations tariff.

→ Access to Ostrava's supercomputing infrastructure can also be obtained through two types of European grant competition announced by the pan-European EuroHPC Joint Undertaking and the PRACE research infrastructure.

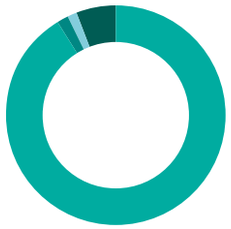
The number of active projects in 2021 was 328. The computational resources these projects were awarded amounted to 282,197,957 core hours. Open Access Grant Competition-based projects were awarded 91% of the computational resources, less than 2% was used by non-commercial projects approved by the IT4Innovations management, and almost 6% of the total was used for the benefit of grant competitions launched by EuroHPC JU and PRACE. The smallest portion of used computational resources, 1.5%, was paid rentals.

Supercomputer utilisation is measured in standard hours of the computer core, i.e. core hours. It is determined as the number of processing units (cores) used to run the computation multiplied by the duration of the job in hours.

↔ Barbora

In the autumn of 2019, the IT4Innovations data room was expanded with another member; the Barbora supercomputer is an extension of the first ever supercomputer at IT4Innovations, Anselm. As with the other Ostrava supercomputers, the name Barbora came as a result of an open competition in which the general public participated.

Distribution of computational resources in 2021



- 91.3% Open Access Grant Competition projects
  257,676,851 of used core hours
- 1.6% Director's Discretion
  4,502,609 of used core hours
- 1.5% Rental of computational resources
  4,237,753 of used core hours
- 5.6% EuroHPC JU and PRACE Grant competitions
  15,780,744 of used core hours

*The used core hours represent the amount of computational resources really used in 2021. The total amount here consists of all research projects that were actually conducted at IT4Innovations this year.

Open Access Grant Competitions 21st, 22nd, 23rd

In 2021, three Open Access Grant Competitions were launched, supporting 188 research projects. Specifically, these were the 21st, 22nd, and 23rd calls. According to the schedule of each call, successful applicants were granted access to computational resources during 2021.

GPU Testing and Benchmarking of the 24th Open Access Grant Competition Special Call was also announced at the end of 2021. Its results will be reported in the 2022 Review together with the standard 24th Open Access Grant Competition.

Projects in the field of materials science were granted the most computational resources, with 66%. Projects in the field of life sciences had the next greatest allocation with 13%, followed by projects in the field of engineering with 9%.

According to the institutions, scientists from VSB - Technical University of Ostrava utilised IT4Innovations supercomputers most (31%), followed by researchers from the Czech Academy of Sciences (26%), and then Charles University and the Czech Technical University in Prague (8% each).

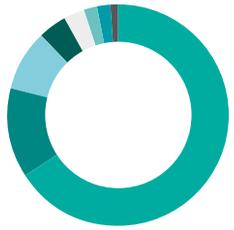
In these three Open Access Grant Competitions, researchers applied for a total of 350 million core hours. In view of the high demand for computational resources compared to the resources offered, the Allocation Committee decided to reduce the allocations of the evaluated projects. The reduction affected all projects proportionally. In total, 292 million core hours were allocated to projects in these rounds of the Public Grant Competition, which is 20% less computing resources than the amount requested.

Comparison of the demand and allocated computational resources within Open Access Grant Competitions (OAGC) in 2018–2021

Year of call announcement – OAGC edition	Number of projects supported	Allocated computational resources (in core hours)	Computational resources required (in core hours)	Users applied for
2018 – 12th – 14th OAGC	164	172,000,000	243,000,000	41% more
2019 – 15th – 17th OAGC	190	227,000,000	348,000,000	53% more
2020 – 18th – 20th OAGC	187	237,000,000	376,000,000	59% more
2021 – 21st – 23rd OAGC	188	292,000,000	350,000,000	20% more

*For the sake of completeness, it should be noted that allocated computational resources differ from used ones. Used computational resources are those which are actually utilised; allocated computational resources indicate how many of them a given project can utilise at most.

Computational resources allocated within the Open Access Grant Competitions in 2021 by scientific discipline



- 66% Material Science
- 13% Biosciences
- 9% Engineering
- 4% Astronomy
- 3% Physics
- 2% Earth sciences
- 2% Computer Science
- 1% Applied mathematics

Computational resources allocated within the Open Access Grant Competitions in 2021 by institution

- 31% VSB - Technical University of Ostrava
- 26% The Czech Academy of Sciences
- 8% Charles University
- 8% The Czech Technical University in Prague
- 5% Masaryk University
- 4% CEITEC
- 4% Palacký University
- 4% The University of Chemistry and Technology in Prague
- 4% The University of Ostrava
- 3% The University of Hradec Králové
- 2% Brno University of Technology
- 1% Others (Tomas Bata University in Zlín, the University of South Bohemia in České Budějovice, the Czech Aerospace Research Centre)

Director's discretion

In 2021, 28 projects using a total of more than 4.5 million core hours were supported within the Director's discretion scheme.

Rental of computational resources

The computational resources used within the paid rental scheme amounted to 4.2 million core hours in 2021.

These were commercial projects of the following companies: AIRMOBIS a.s., Bonmedix s.r.o., DHI a.s., Sotio a.s., Ullmanna s.r.o., the Institute for Forest Management Brandýs nad Labem, and Varroc Lighting systems, s.r.o.

EuroHPC JU and PRACE grant competitions

In 2021, nearly 16,000,000 core hours were used within these competitions, shared by 9 projects. Of these, 5 projects (486,372 core hours) were carried out under the EuroHPC JU call and 4 projects (15,294,372 core hours) under PRACE.

Users of computational resources

The number of active users of IT4Innovations' computing infrastructure increased by 42% year-on-year to 863 in 2021. The IT4Innovations Technical Support provided to its users received a total of 1,608 queries and requests. The internal response time (24 hours for the first response) was met for 99.7% of the suggestions. The internal closure time, which must not exceed 30 days, was observed in 94.6% of the queries.

5

Research and Development

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

IT4Innovations is a research and development centre with strong international links, and as such it actively participates in all activities of the EuroHPC Joint Undertaking and in a number of prestigious international organisations (PRACE, ETP4HPC, I4MS, EUDAT, BDVA/DAIRO, EOSC). In 2021, it participated in sixteen international projects funded by Horizon 2020 and coordinated one of these projects, LEXIS (Large-scale Execution for Industry & Society). IT4Innovations is also a National Competence Centre in HPC within the European EuroCC project and a member of the H2020 POP2 Centre of Excellence.

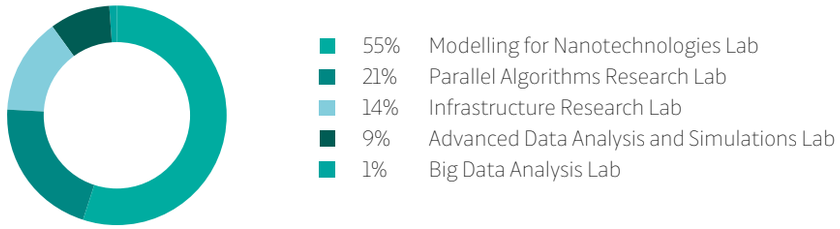
Moreover, IT4Innovations is involved in development of the European Space Agency (ESA) funded Urban Thematic Exploitation Platform, and has in the past participated in a number of projects supported by the FP7 and H2020 programmes such as PRACE, EXA2CT, HARPA, ExCAPE, ANTAREX, READEX, SESAME NET, and many others.

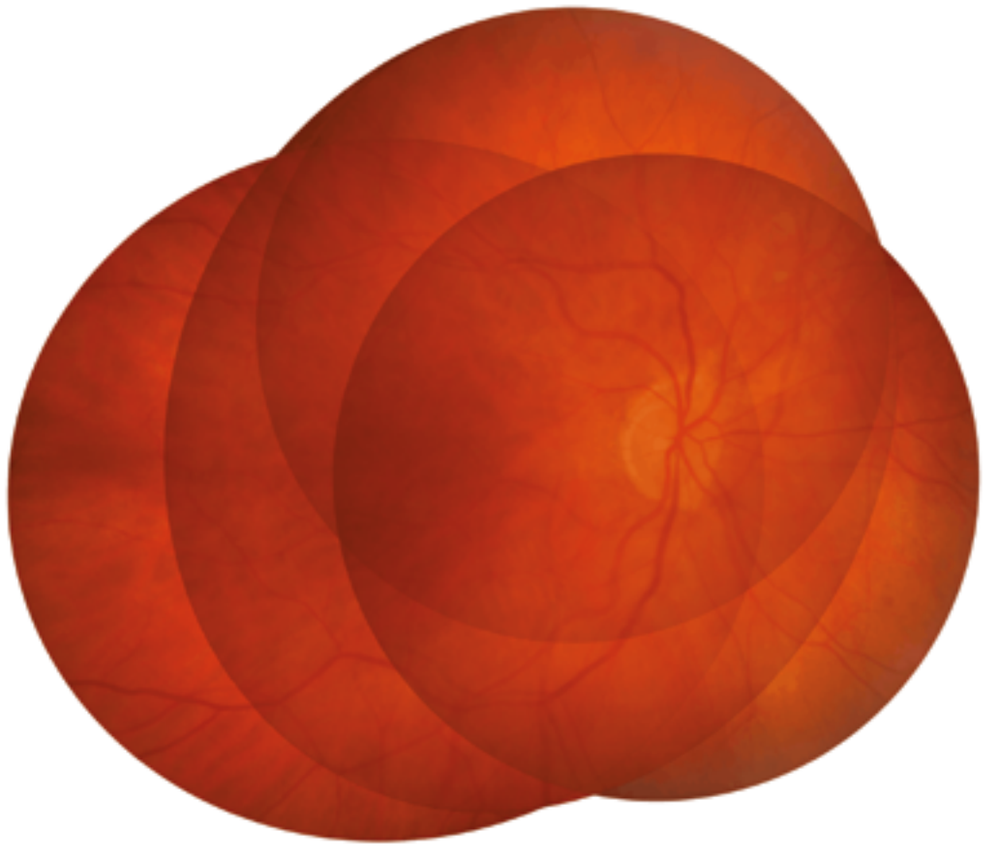
IT4Innovations research activities are carried out across five laboratories:

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

IT4Innovations research labs were awarded computational resources for 59 research projects within the 21st to 23rd Open Access Grant Competition, with over 86 million core hours allocated, representing 29% of the total allocation of all supported projects. The majority of the projects were submitted by the researchers from the Advanced Data Analysis and Simulations Lab, and the majority of the computational resources were awarded to the Modelling for Nanotechnologies Lab.

Utilisation of IT4Innovations computational resources by research labs in 2021 (assigned allocations)





↔ Improving Retinal Screenings of Patients

The aim of the project IT4Innovations participates in collaboration with the Bonmedix company is to develop a new service that enables a multifold increase in preventive and control screenings of the ocular fundus (retina) in order to detect diseases or progression as early as possible and thus reduce the subsequent costs of further treatment of patients, which will then be certified as a medical device.

Research and Development Flagships

In 2021, IT4Innovations research and development continued to be conducted within the flagships representing IT4Innovations scientific excellence, which were selected by the Research Council of the IT4Innovations Centre of Excellence in 2018.

ESPRESO, Highly Parallel Finite Element Package for Engineering Simulations

→ Principal investigator: Dr Tomáš Brzobohatý

The latest technological advances in computing have brought a significant change in the concept of new product design, production control, and autonomous systems. In the last few years, we have been witnessing a significant and considerable transition to virtual prototyping, and gradually increasing pressure to integrate large parts of the industrial sector into the fourth industrial revolution. The main objective of the flagship is to create a robust open-source package (ESPRESO) applicable to a wide range of complex engineering simulations in areas such as mechanical engineering, civil engineering, biomechanics, and the energy industry. The open-source approach allows automatised simulation chains, based on HPC-as-a-service, such as automatised systems for shape or topological optimisation, which will be created on the top of the ESPRESO framework. In the development of new ESPRESO library components, highly scalable methods are used to take full advantage of the computational capacity of state-of-the-art supercomputers.

Material Design – Towards Reality via Exascale Computing

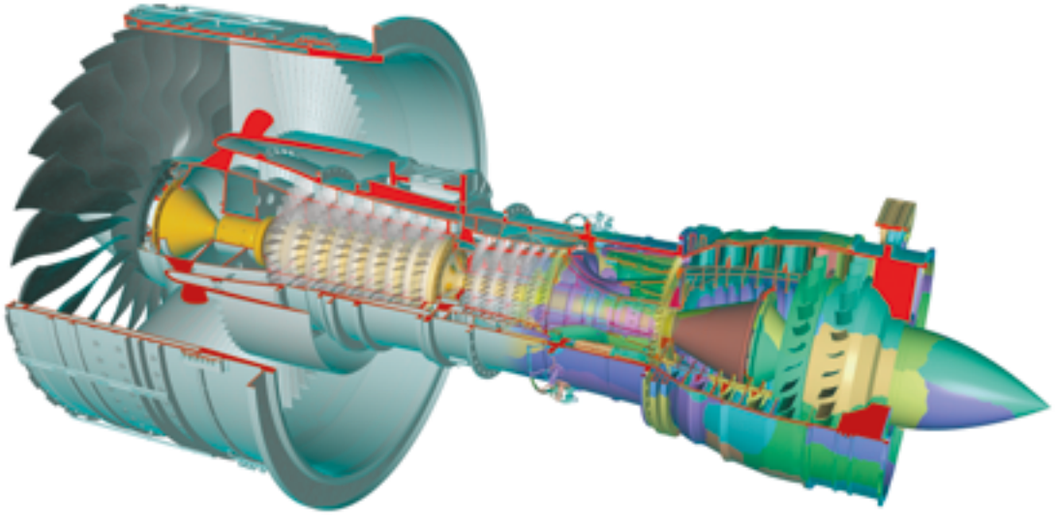
→ Principal investigator: Dr Dominik Legut

As advances in HPC have been made, simulation of material behaviour has come to play a key role in our lives. This fact became even more pronounced once there was a way to perform quantum mechanical calculations to obtain the electronic structure of materials and their behaviour, and link it to many physical and chemical properties. First-principles (ab initio) calculations at present are the parameter-free approach for i) verification of experiments ii) simulating conditions or calculating material properties that are not directly accessible or measurable, and iii) designing novel materials. Within the flagship we address fundamental and state-of-the-art topics like the design of nuclear fuel materials from radioactive compounds for generation IV nuclear reactors, ultrafast magnetisation dynamics for novel data storage, complex spintronic devices exploiting multiferroicity, and engineering applicable materials at finite temperatures and pressures, e.g., novel permanent magnets.

HPC platforms for scientific workflow execution

→ Principal investigators: Dr Jan Martinovič, Dr Stanislav Böhm and Dr Václav Svatoň

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



↔ Numerical simulations

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

Summary of Science and Research Results in 2021

This subsection presents the results of IT4Innovations science and research in 2021.

Science and research results in 2021 based on the RIV 2017+ Methodology

Summary of the achieved IT4Innovations science and research results in 2021

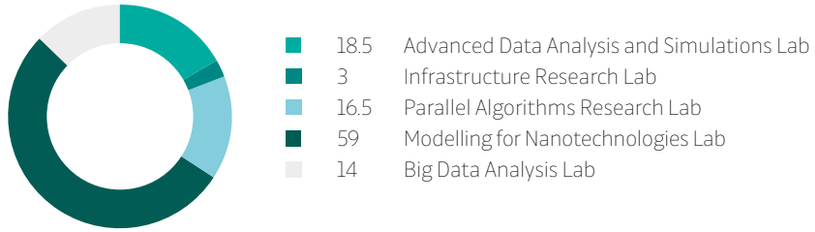
Results classified based on the RIV 2017+ Methodology	Achieved results
Jimp – article in the Web of Science database	106
JSC – article in the SCOPUS database	5
Jost – other reviewed articles	1
B – reviewed publication	0
C – chapter in a reviewed publication	1
D – section in a proceeding	21
P – patent	0
F – utility model, industrial design	1
Z – semioperation, verified technology	0
G – prototype, functional sample	2
H – results reflected in norms and directives	0
N – methodology, specialised map	0
R – software	18
V – research report	0

Jimp and Jsc Journal Publications in 2021 by individual labs and ranking

Jimp and Jsc Journal Publications in 2021 by individual labs and ranking	D1	Q1\D1	Q2	Q3	Q4	Total
Advanced Data Analysis and Simulations Lab	6	7	4.5	0	1	18.5
Infrastructure Research Lab	1	1	1	0	0	3
Parallel Algorithms Research Lab	5	5	3.5	3	0	16.5
Modelling for Nanotechnologies Lab	32	24	3	0	0	59
Big Data Analysis Lab	4	4	4	2	0	14
Total	48	41	16	5	1	111

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

Number of journal publications in 2021 by individual labs



List of D1 publications sorted by individual labs

Advanced Data Analysis and Simulations Lab

- Zitzlsberger Georg, Podhorányi Michal, Svatoň Václav, Lazecký Milan, Martinovič Jan. *Neural Network-Based Urban Change Monitoring with Deep-Temporal Multispectral and SAR Remote Sensing Data.* Remote Sensing, vol. 13, is. 15, 2021. DOI 10.3390/rs13153000, IF 4.848 (JIMP D1).

- Vitali E., Gadioli D., Palermo G., Golasowski Martin, Bispo J., Pinto P., Martinovič Jan, Slaninová Kateřina, Cardoso J., Silvano C. *An Efficient Monte Carlo-based Probabilistic Time-Dependent Routing Calculation Targeting a Server-Side Car Navigation System.* IEEE Transactions on Emerging Topics in Computing, vol. 9, is. 2, p. 1006–1019, 2021. DOI 10.1109/TETC.2019.2919801, IF 7.691 (JIMP D1).

- Lampart Marek, Zapoměl Jaroslav. *Motion of an Unbalanced Impact Body Colliding with a Moving Belt.* Mathematics, vol. 9, is. 9, 2021. DOI 10.3390/math9091071, IF 2.258 (JIMP D1).

- Danca Marius-F., Lampart Marek. *Hidden and self-excited attractors in a heterogeneous Cournot oligopoly model.* Chaos, Solitons & Fractals, January 2021.

- Tomčala Jiří. *Towards optimal supercomputer energy consumption forecasting method.* Mathematics, vol. 142, is. January 2021. DOI 10.1016/j.chaos.2020.110371, IF 5.944 (JIMP D1).

- Lampart Marek, Zapoměl Jaroslav. *Chaos identification of a colliding constrained body on a moving belt.* Nonlinear Dynamics, vol. 1, is. 104, p. 2723–2732, 2021. DOI 10.1007/s11071-021-06383-6, IF 5.022 (JIMP D1).

Infrastructure Research Lab

- Jaroš Milan, Říha Lubomír, Strakoš Petr, Špeťko Matej. *GPU Accelerated Path Tracing of Massive Scenes.* ACM Transactions on Graphics, vol. 40, is. 2, 2021. DOI 10.1145/3447807, IF 5.414 (JIMP D1).

Parallel Algorithms Research Lab

→ Zapletal Jan, Watschinger Raphael, Of Günther, Merta Michal. *Semi-analytic integration for a parallel space-time boundary element method modelling the heat equation.* Computers & Mathematics with Applications, vol. 103, is. 1, p. 156–170, December 2021. DOI 10.1016/j.camwa.2021.10.025, IF 3.476 (JIMP D1).

→ Dostál Zdeněk, Brzobohatý Tomáš, Vlach Oldřich. *Schur complement spectral bounds for large hybrid FETI-DP clusters and huge three-dimensional scalar problems.* Journal of Numerical Mathematics, vol. 29, is. 4, p. 289–306, 2021. DOI 10.1515/jnma-2020-0048, IF 3.778 (JIMP D1).

→ Dostál Zdeněk, Horák David, Brzobohatý Tomáš, Vodstrčil Petr. *Bounds on the spectra of Schur complements of large H-TFETI-DP clusters for 2D Laplacian.* Numerical Linear Algebra with Applications, vol. 28, is. 2, 2021. DOI 10.1002/nla.2344, IF 2.109 (JIMP D1).

→ Haslinger Jaroslav, Kučera Radek, Motyčková Kristina, Šátek Václav. *Numerical modeling of the leak through semipermeable walls for 2D/3D Stokes flow: experimental scalability of dual algorithms.* Mathematics, vol. 9, is. 22, 2021. DOI 10.3390/math9222906, IF 2.258 (JIMP D1).

→ Šofer Michal, Šofer Pavel, Ferfecki Petr, Molčan Michal, Stryja Jakub. *Lamb Wave Mode Scattering Analysis on Adhesively Bonded Single Lap Joint using Modal Decomposition Method.* Applied Mathematical Modelling, vol. 89, is. 08-2020, p. 413–427, 2021. DOI 10.1016/j.apm.2020.08.017, IF 5.129 (JIMP D1).

Modelling for Nanotechnologies Lab

→ Wdowik Urszula Danuta, Buturlim V., Havela L., Legut Dominik. *Effect of carbon vacancies and oxygen impurities on the dynamical and thermal properties of uranium monocarbide.* Journal of Nuclear Materials, vol. 545, March 2021. DOI 10.1016/j.jnucmat.2020.152547, IF 2.936 (JIMP D1).

→ Mallada Benjamin, Blonski Piotr, Langer Rostislav, Jelinek Pavel, Otyepka Michal, de la Torre Bruno. *On-Surface Synthesis of One-Dimensional Coordination Polymers with Tailored Magnetic Anisotropy.* ACS applied materials & interfaces, vol. 13, is. 27, p. 32393–32401, 2021. DOI 10.1021/acsami.1c04693, IF 9.229 (JIMP D1).

→ Legut Dominik, Kadzielawa Andrzej Piotr, Pánek Petr, Marková Kristýna, Váňová Petra, Konečná Kateřina, Langová Šárka. *Inhibition of steel corrosion with imidazolium-based compounds – Experimental and theoretical study.* Corrosion Science, vol. 191, is. October 2021, p. 109716, 2021. DOI 10.1016/j.corsci.2021.109716, IF 7.205 (JIMP D1).

→ Nguyen-Huu N., Pištora Jaromír, Čada Michal, Nguyen-Thoi T., Ma Y., Yasumoto K., Rahman B. M. A., Wu Q., Ma Y., Ngo Q. H., Jie L., Maeda H. *Ultra-wide Spectral Bandwidth and Enhanced Absorption in a Metallic Compound Grating Covered by Graphene Monolayer.* IEEE Journal on Selected Topics in Quantum Electronics, vol. 27, is. 1, 2021. DOI 10.1109/JSTQE.2020.2984559, IF 4.544 (JIMP D1).

→ Otyepková E., Skladanová K., Pykal M., Blahová Prudilová B., Kašlík J., Čépe K., Banáš P., Lazar P., Otyepka Michal. *Molecular insights from theoretical calculations explain the differences in affinity and diffusion of airborne contaminants on surfaces of hBN and graphene.* Applied Surface Science, vol. 565, is. November 2021. DOI 10.1016/j.apsusc.2021.150382, IF 6.707 (JIMP D1).

→ Ma Youqiao, Li Jinhua, Han Zhanghua, Maeda Hiroshi, Pištora Jaromír. *All-Dielectric Graphene-induced T-Slot Waveguide Electro-Optic Modulator With Polarization-Independent Operation.* IEEE Journal on Selected Topics in Quantum Electronics, vol. 27, is. 3, 2021. DOI 10.1109/JSTQE.2021.3050569, IF 4.544 (JIMP D1).

→ Wei B., Legut Dominik, Sun S., Wang H. T., Shi Z. Z., Zhang H. J., Zhang R. F. *An improved electrochemical model for strain dependent electrochemical polarization and corrosion kinetics.* Materials and Design, vol. 202, 2021. DOI 10.1016/j.matdes.2021.109555, IF 7.991 (JIMP D1).

→ Shen X. P, Yao B. N, Liu Z. R, Legut Dominik, Zhang H. J, Zhang R. F. *Mechanistic insights into interface-facilitated dislocation nucleation and phase transformation at semicoherent bimetal interfaces.* International Journal of Plasticity, vol. 146, 2021. DOI 10.1016/j.ijplas.2021.103105, IF 7.081 (JIMP D1).

→ Mallada B., Gallardo A., Lamanec Maximilián, de la Torre B., Špirko V., Hobza Pavel, Jelinek P. *Real-space imaging of anisotropic charge of σ-hole by means of Kelvin probe force microscopy.* Science, vol. 374, is. 6569, p. 863–867, 2021.DOI 10.1126/science.abk1479, IF 47.728 (JIMP D1).

→ Paloncýová M., Čechová P., Šrejber M., Kührová P., Otyepka Michal. *Role of Ionizable Lipids in SARS-CoV-2 Vaccines As Revealed by Molecular Dynamics Simulations: From Membrane Structure to Interaction with mRNA Fragments.* Journal of Physical Chemistry Letters, vol. 12, is. 45, p. 11199–11205, 2021. DOI 10.1021/acs.jpclett.1c03109, IF 6.475 (JIMP D1).

→ Kiehbadroudinezhad Mohammadali, Rajabipour Ali, Čada Michal, Khanali Majid. *Modeling, design, and optimization of a cost-effective and reliable hybrid renewable energy system integrated with desalination using the division algorithm.* International Journal of Energy Research, vol. 45, is. 1, p. 429–452, 2021. DOI 10.1002/er.5628, IF 5.164 (JIMP D1).

→ Lo R., Manna D., Lamanec Maximilián, Wang W., Bakandritsos Aristeidis, Dračínský M., Zbořil Radek, Nachtigallová Dana, Hobza Pavel. *Addition Reaction between Piperidine and C60to Form 1,4-Disubstituted C60Proceeds through van der Waals and Dative Bond Complexes: Theoretical and Experimental Study.* Journal of the American Chemical Society, vol. 143, is. 29, p. 10930–10939, 2021. DOI 10.1021/jacs.1c01542, IF 15.419 (JIMP D1).

↔ At the beginning of 2021, the first-ever Ostrava supercomputer, Anselm, was shut down. It is now on display in the Science and Technology Centre in Dolní Vítkovice in Ostrava.

→ de la Cruz Artorix, Qasymeh Montasir, Pištora Jaromír, Čada Michal. *Electronically controlled polarization beat length in Kerr nonlinear media.* Results in Physics, vol. 25, is. June 2021. DOI 10.1016/j.rinp.2021.104232, IF 4.476 (JIMP D1).

→ Gu Yitao, Wei Bo, Legut Dominik, Fu Zhongheng, Du Shiyu, Zhang Haijun, Francisco Joseph S, Zhang Ruifeng. *Single Atom-Modified Hybrid Transition Metal Carbides as Efficient Hydrogen Evolution Reaction Catalysts.* Advanced Functional Materials, vol. 31, is. 43, 2021. DOI 10.1002/adfm.202104285, IF 18.808 (JIMP D1).

→ Wei Bo, Fu Zhongheng, Legut Dominik, Germann Timothy C, Du Shiyu, Zhang Haijun, Francisco Joseph S, Zhang Ruifeng. *Rational Design of Highly Stable and Active MXene-Based Bifunctional ORR/OER Double-Atom Catalysts.* Advanced Materials, vol. 33, is. 40, 2021. DOI 10.1002/adma.202102595, IF 30.849 (JIMP D1).

→ Wei B., Legut Dominik, Sun S., Wang H. T., Shi Z. Z., Zhang H. J., Zhang R. F. *Synergistic effect of solute and strain on the electrochemical degradation in representative Zn-based and Mg-based alloys.* Corrosion Science, vol. 188, p. 109539, 2021. DOI 10.1016/j.corsci.2021.109539, IF 7.205 (JIMP D1).

→ Cruz Artorix de la, Čada Michal, Pištora Jaromír, Diaz-Chang Tamara. *Asymptotic variational approach to study light propagation in a nonlocal nonlinear medium.* Results in Physics, vol. 27, 2021. DOI 10.1016/j.rinp.2021.104536, IF 4.476 (JIMP D1).

→ Saini Haneesh, Kallem Parashuram, Otyepkova Eva, Geyer Florian, Schneemann Andreas, Ranc Vaclav, Banat Fawzi, Zbořil Radek, Otyepka Michal, Fischer Roland A, Jayaramulu Kolleboyina. *Two-dimensional MOF-based liquid marbles: surface energy calculations and efficient oil-water separation using a ZIF-9-III@PVDF membrane*. Journal of Materials Chemistry A, vol. 9, is. 41, p. 23651–23659, 2021. DOI 10.1039/d1ta05835e, IF 12.732 (JIMP D1).

→ Saini H., Srinivasan N., Šedajová V., Majumder M., Dubal D.P., Otyepka Michal, Zbořil Radek, Kurra N., Fischer R.A., Jayaramulu K. *Emerging MXene@Metal-Organic Framework Hybrids: Design Strategies toward Versatile Applications.* ACS Nano, vol. 15, is. 12, p. 18742–18776, 2021. DOI 10.1021/acsnano.1c06402, IF 15.881 (JIMP D1).

→ Olšovská Eva, Tokarský Jonáš, Michalička Jan, Mamulová Kutláková Kateřina. *Simple and fast method for determination of preferred crystallographic orientation of nanoparticles: A study on ZnS/kaolinite nanocomposite*. Applied Surface Science, vol. 544, 2021. DOI 10.1016/j.apsusc.2021.148966, IF 6.707 (JIMP D1).

→ Ma Youqiao, Li Jinhua, Čada Michal, Bian Yusheng, Han Zhanghua, Ma Yuan, Iqbal Muddassir, Pištora Jaromír. *Plasmon Generation and Routing in Nanowire-Based Hybrid Plasmonic Coupling Systems With Incorporated Nanodisk Antennas*. IEEE Journal on Selected Topics in Quantum Electronics, vol. 27, is. 1, 2021. DOI 10.1109/JSTQE.2020.3008651, IF 4.544 (JIMP D1).

→ Tokarčíková Michaela, Seidlerová Jana, Motyka Oldřich, Životský Ondřej, Drobíková Klára, Gabor Roman. *Experimental verification of regenerable magnetically modified montmorillonite and its application for heavy metals removal from metallurgical waste leachates*. Journal of Water Process Engineering, vol. 39, is. February, 2021. DOI 10.1016/j.jwpe.2020.101691, IF 5.485 (JIMP D1).

→ Nieves Cordones Pablo, Arapan Sergiu, Zhang S.H., Kadzielawa Andrzej Piotr, Zhang R.F., Legut Dominik. *MAELAS: MAgneto-ELAStic properties calculation via computational high-throughput approach.* Computer Physics Communications, vol. 264, is. July 2021. DOI 10.1016/j.cpc.2021.107964, IF 4.39 (JIMP D1).

→ Ma Chunrong, Hou Yang, Jiang Kai, Zhao Long, Olsen Tristan, Fan Yanchen, Jiang Jiali, Xu Zhixin, Ma ZiFeng, Legut Dominik, Xiong Hui, Yuan Xian-Zheng. *In situ cross-linking construction of 3D mesoporous bimetallic phosphide-in-carbon superstructure with atomic interface toward enhanced sodium ion storage performance.* Chemical engineering journal, vol. 413, is. June 2021. DOI 10.1016/j.cej.2020.127449, IF 13.273 (JIMP D1).

→ Wang C. J, Liu Z. R, Yao B. N, Kong X. F, Legut Dominik, Zhang R. F, Deng Y. *Effects of hydrogen clusters on interface facilitated plasticity at semi-coherent bimetal interfaces.* Scripta materialia, vol. 190, p. 63–68, 2021. DOI 10.1016/j.scriptamat.2020.08.031, IF 5.611 (JIMP D1).

→ Mayorga-Burrezo Paula, Munoz Jose, Zaoralova Dagmar, Otyepka Michal, Pumera Martin. *Multiresponsive 2D Ti3C2Tx MXene via Implanting Molecular Properties.* ACS Nano, vol. 15, is. 6, p. 10067–10075, 2021. DOI 10.1021/acsnano.1c01742, IF 15.881 (JIMP D1).

→ Vermisoglou E. C., Jakubec P., Bakandritsos Aristeidis, Kupka V., Pykal M., Šedajová V., Vlček J., Tomanec O., Scheibe M., Zbořil Radek, Otyepka Michal. *Graphene with Covalently Grafted Amino Acid as a Route Toward Eco-Friendly and Sustainable Supercapacitors.* ChemSusChem, vol. 14, is. 18, p. 3904–3914, 2021. DOI 10.1002/cssc.202101039, IF 8.928 (JIMP D1).

→ Jayaramulu Kolleboyina, Esclance DMello Marilyn, Kesavan Kamali, Schneemann Andreas, Otyepka Michal, Kment Štěpán, Narayana Chandrabhas, Kalidindi Suresh Babu, Varma Rajender S, Zbořil Radek, Fischer Roland A. *A multifunctional covalently linked graphene-MOF hybrid as an effective chemiresistive gas sensor.* Journal of Materials Chemistry A, vol. 9, is. 32, p. 17434–17441, 2021. DOI 10.1039/d1ta03246a, IF 12.732 (JIMP D1).

→ Zhang Y., Melchionna M., Medved M., Błoński P, Steklý T., Bakandritsos Aristeidis, Kment Štěpán, Zbořil Radek, Otyepka Michal, Fornaserio P., Naldoni A. *Enhanced On-Site Hydrogen Peroxide Electrosynthesis by a Selectively Carboxylated N-Doped Graphene Catalyst.* ChemCatChem, vol. 13, is. 20, p. 4372–4383, 2021. DOI 10.1002/cctc.202100805, IF 5.686 (JIMP D1).

→ Majumder M., Saini H., Dědek I., Schneemann A., Chodankar N. R., Ramarao V., Santosh

M. S. , Nanjundan A.K., Kment Štěpán, Dubal D., Otyepka Michal, Zbořil Radek, Jayaramulu K. Rational Design of Graphene Derivatives for Electrochemical Reduction of Nitrogen to Ammonia. ACS Nano, vol. 15, is. 11, p. 17275–17298, 2021. DOI 10.1021/acsnano.1c08455, IF 15.881 (JIMP D1).

→ Alzate-Carvajal N., Park J., Pykal M., Lazar P., Rautela R., Scarfe S., Scarfe L., Ménard J.-M., Otyepka Michal, Luican-Mayer A. *Graphene Field Effect Transistors: A Sensitive Platform for Detecting Sarin.* ACS applied materials & interfaces, vol. 13, is. 51, p. 61751–61757, 2021. DOI 10.1021/acsami.1c17770, IF 9.229 (JIMP D1).

→ Dolezal Petr, Cejpek Petr, Tsutsui Satoshi, Kaneko Koji, Legut Dominik, Carva Karel, Javorsky Pavel. *Lattice dynamics in CePd2Al2 and LaPd2Al2.* Scientific Reports, vol. 11, is. 1, 2021. DOI 10.1038/s41598-021-99904-7, IF 4.38 (JIMP D1).

Big Data Analysis Lab

→ Tin P. T., Phan V.-D., Nguyen T. N., Tu L.-T., Minh B.V., Vozňák Miroslav, Fazio Peppino. *Outage analysis of the power splitting based underlay cooperative cognitive radio networks.* Sensors, vol. 21, is. 22, 2021. DOI 10.3390/s21227653, IF 3.576 (JIMP D1).

→ Ševčík Lukáš, Vozňák Miroslav. *Adaptive reservation of network resources according to video classification scenes.* Sensors, vol. 21, is. 6, p. 1-31, 2021. DOI 10.3390/s21061949, IF IF 3.576 (JIMP D1).

→ Růžičková Kateřina, Růžička Jan, Bitta Jan, Chudasová Gabriela. *A new GIS-compatible methodology for visibility analysis in digital surface models of earth sites.* Geoscience Frontiers, vol. 12, is. 4, 2021. DOI 10.1016/j.gsf.2020.11.006, IF 6. 853 (JIMP D1).

→ Gens Antonio, Alcoverro Jordi, Blaheta Radim, Hasal Martin, Michalec Zdenek, Takayama Yusuke, Lee Changsoo, Lee Jaewon, Kim Geon Young, Kuo Chia-Wei, Kuo Wan-Jung, Lin Chung-Yi. *HM and THM interactions in bentonite engineered barriers for nuclear waste disposal.* International journal of rock mechanics and mining sciences, vol. 137, is. January 2021. DOI 10.1016/j.ijrmms.2020.104572, IF 7.135 (JIMP D1).

Latest evaluation results based on the M1 RIV 2017+ Methodology module evaluated by a score from 1 to 3

Advanced Data Analysis and Simulations Lab

→ Kožusznik Jan, Bainar Petr, Klímová Jana, Krumnikl Michal, Moravec Pavel, Svatoň Václav, Tomančák Pavel. *SPIM workflow manager for HPC.* Bioinformatic vol. 35, is. 19, p. 3875–3876, 2019. DOI 10.1093/bioinformatics/btz140, IF 6.937 (JIMP D1).

Infrastructure Research Lab

→ Jaroš Milan, Strakoš Petr, Říha Lubomír. CyclesPhi renderer. 023/09-12-2019_SW, 2019.

→ Meca Ondřej, Říha Lubomír, Brzobohatý Tomáš. Knihovna pro paralelní převod mezi formáty konečněprvkových síti MESIO. 021/09-12-2019_SW, 2019.

→ Peterek Ivo, Beseda Martin, Vysocký Ondřej, RADAR visualizer, 022/09-12-2019_SW, 2019.

Parallel Algorithms Research Lab

→ Koubová Lenka, Janas Petr, Markopoulos Alexandros, Krejsa Martin. *Nonlinear analyses of steel beams and arches using virtual unit moments and effective rigidity.* Steel and Composite Structures, vol. 33, is. 5, p. 755–765, 2019. DOI 10.12989/scs.2019.33.5.755, IF 5.733 (JIMP D1).

→ Van de Steen Cyril, Benhenni Malika, Kalus René, Ćosić Rajko, Gadea Florent Xavier, Yousfi Mohammed. *Mobility and dissociation of electronically excited Kr-2(+) ions in cold krypton plasma.* Plasma Sources Science and Technology, vol. 28, is. 9, 2019. DOI 10.1088/1361-6595/ab3a17, IF 3.584 (JIMP Q1).

→ Dohr Stefan, Zapletal Jan, Of Gunther, Merta Michal, Kravčenko Michal. *A parallel space-time boundary element method for the heat equation.* Computers & Mathematics with Applications, vol. 78, is. 9, p. 2852–2866, 2019. DOI 10.1016/j.camwa.2018.12.031, IF 3.476 (JIMP D1).

→ Kravčenko Michal, Merta Michal, Zapletal Jan. *Distributed fast boundary element methods for Helmholtz problems.* Applied Mathematics and Computation, vol. 362, is. December 2019, p. 1–15, 2019. DOI 10.1016/j.amc.2019.06.017, IF 4.091 (JIMP D1).

→ Zapletal Jan, Bouchala Jiří. *Shape optimization and subdivision surface based approach to solving 3D Bernoulli problems.* Computers & Mathematics with Application, vol. 78, is. 9, p. 2911–2932, 2019. DOI 10.1016/j.camwa.2019.02.015, IF 3.476 (JIMP D1).

→ Van de Steen Cyril, Benhenni Malika, Kalus René, Ćosić Rajko, Illésová Silvie, Gadea Florent Xavier, Yousfi Mohammed. *Cross-sections, transport coefficients and dissociation rate constants for Kr-2(+) molecular ion interacting with Kr.* Plasma Sources Science and Technology, vol. 28, is. 3, 2019. DOI 10.1088/1361-6595/aaebe0, IF 3.584 (JIMP Q1).

→ Dostál Zdeněk, Vlach Oldřich, Brzobohatý Tomáš. *Scalable TFETI based algorithm with adaptive augmentation for contact problems with variationally consistent discretization of contact conditions.* Finite Elements in Analysis and Design, vol. 156, p. 34–43, 2019. DOI 10.1016/j.finel.2019.01.002, IF 2.972 (JIMP Q1).

Modelling for Nanotechnologies Lab

→ Xiao Jiewen, Zhou Guangmin, Chen Hetian, Feng Xiang, Legut Dominik, Fan Yanchen, Wang Tianshuai, Cui Yi, Zhang Qianfan. *Elaboration of Aggregated Polysulfide Phases: From Molecules to Large Clusters and Solid Phases.* Nano Letters, vol. 19, is. 10, p. 7487–7493, 2019. DOI 10.1021/acs.nanolett.9b03297, IF 11.189 (JIMP D1).

→ Chen Hetian, Handoko Albertus D, Xiao Jiewen, Feng Xiang, Fan Yanchen, Wang Tianshuai, Legut Dominik, Seh Zhi Wei, Zhang Qianfan. *Catalytic Effect on CO2 Electroreduction by Hydroxyl-Terminated Two-Dimensional MXenes.* ACS applied materials & interfaces, vol. 11, is. 40, p. 36571–36579, 2019. DOI 10.1021/acsami.9b09941, IF 9.229 (JIMP Q1).

→ Wang T., Zhai P., Legut Dominik, Wang L., Liu X., Li B., Dong C., Fan Y., Gong Y., Zhang Q. *S-Doped Graphene-Regional Nucleation Mechanism for Dendrite-Free*

Lithium Metal Anodes. Advanced Energy Materials, vol. 9, is. 24, 2019. DOI 10.1002/aenm.201804000, IF 20.368 (JIMP D1).

Big Data Analysis Lab

→ Skanderová Lenka, Fabián Tomáš, Zelinka Ivan. *Self-adapting self-organizing migrating algorithm*. Swarm and Evolutionary Computation, vol. 51, 2019. DOI 10.1016/j.swevo.2019.100593, IF 7.177 (JIMP D1).

Number of results by individual labs

1	Advanced Data Analysis and Simulations Lab
3	Infrastructure Research Lab
7	Parallel Algorithms Research Lab
3	Modelling for Nanotechnologies Lab
1	Big Data Analysis Lab

↔ Visit from the European Commission

On 17th July, Frans Timmermans, Vice-President of the European Commission, visited IT4Innovations to chair a discussion on the green future of Europe. As part of the programme, he also took the excursion of the IT4Innovations data room.

Advanced Data Analysis and Simulations Lab

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

Head of lab: Dr Jan Martinovič
Number of employees: 40.63 FTE

Significant activities

- Three EuroHPC JU projects were successfully started: LIGATE, ACROSS, and IO-SEA, coordinated by the pharmaceutical Dompé company, the research LINKS organisation, and the research CEA organisation, respectively.
- A new version of HEAppE Middleware was released enabling long term execution, generic command templates, and OpenMPI & MPI support, and with various fixes and security improvements. A new HEAppE website (heappe.eu) was released.
- Complex workflow orchestration on both HPC and Cloud platforms has been successfully implemented in the LEXIS Platform as a main goal of the LEXIS H2020 Project.
- The work on HyperQueue has successfully started, and it is actively used by both internal and external users on IT4Innovations infrastructure. HyperQueue is also considered by LUMI as a main tool for subnode scheduling.
- A simulation of a vaccination centre throughput was created and used for the design of a vaccination centre in Ostrava.
- The new study subject 'Introduction to Quantum Computing' focusing on MSc students has been introduced at VSB-TUO.
- Martin Golasowski won the bronze award in the Joseph Fourier Prize competition for his project focused on the optimisation of urban transport using intelligent navigation service.
- Georg Zitzlsberger obtained two NVIDIA Deep Learning Institute (DLI) instructor certificates: Building Transformer-Based Natural Language Processing Applications and Fundamentals of Deep Learning.

Infrastructure Research Lab

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

Head of lab: Dr Lubomír Říha
Number of employees: 13.10 FTE

Significant activities

- The registered MESIO software for parallel loading and conversion of databases of unstructured networks received a high rating (2) in the RIV 2017+ methodology.
- A new version of the CyclesPhi renderer software with the unique feature of rendering huge scenes in the shared memory of multiple GPU accelerators was created and registered.
- The creation of a Medical-as-a-Service for cooperation with University Hospital Ostrava for CT image segmentation with the possibility of re-learning and refining models based on user feedback.
- The preparation and organisation of two courses on MPI for beginners and advanced users within the PRACE Training Centre, and of a full-day course on CUDA programming within the international SCtrain project.
- The implementation and running of two Master's degree courses at the Department of Applied Mathematics, the Faculty of Electrical Engineering and Computer Science at VSB – Technical University of Ostrava.
- Jakub Homola was awarded the Prof. Babuška Prize for outstanding work in computer science for the year 2021 by an expert jury on the basis of his master's thesis, for which he used our supercomputers.
- The cooperation within the international Energy Efficient High Performance Computing Working Group, which is dedicated to measuring, managing, and optimising the power consumption of computing infrastructures.

Parallel Algorithms Research Lab

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

Head of lab: Dr Tomáš Karásek
Number of employees: 22.59 FTE

Significant activities

- In 2021 cooperation with Siemens s.r.o. (Frenštát branch of electrical engines) and SVS FEM s.r.o. continued on the project 'Digital twin product' at Siemens manufacturing plants.

- Continuation of the project 'Inlet and outlet objects of pumping and turbine stations'. In this project, we cooperated with SIGMA Research and Development Institute, s.r.o., Centre for hydraulic research, s.r.o., and the Institute of Thermomechanics of the CAS, v. v. i.

- The development of libraries for molecular simulations and their use in computations continued: MULTIDYN. Work continued on linking the two libraries, LIB4NEURO and NEURON4DYN (representation of molecular interactions using artificial neural networks).

Modelling for Nanotechnologies Lab

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

Head of lab: Prof. Michal Otyepka
Number of employees: 15.78 FTE

Significant activities

- Collaboration on a breakthrough discovery published in the journal Science: the observation of the inhomogeneous electron charge distribution on an atom, i.e. sigma-hole. The discovery confirmed a 30-year-old theoretical prediction and further demonstrated the possibility of achieving “subatomic” resolution by scanning probe microscopy.

- The design and computer simulations of anisotropic nanostructured spin lasers with ultrafast polarisation dynamics up to THz frequencies.

- The modelling of corrosion inhibition and electrochemical polarisation on pure iron and Mg- and Zn-based alloys by imidazolium ions, dissolved transitive metals, and mechanical stress.

- Collaboration on the development of a single-atom catalyst on the surface of novel functionalised 2D materials (nitrides and carbides of transitive metals) to improve the efficiency of the hydrogen evolution reaction. The result was published in the Advanced Functional Materials journal.

- The development of a code to determine the magnetostrictive and magneto-elastic coefficients of 3D ferromagnetic materials based on ab initio calculations.

↔ The Visualisation and Virtual Reality Labs are used to visualise 3D content using the latest technologies available in the areas of large-scale 3D projection and virtual reality.

Big Data Analysis Lab

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

Head of lab: Prof. Miroslav Vozňák
Number of employees: 4.81 FTE

Significant activities

- The first national, but also international intercity quantum key transfer in the Czech Republic, namely between Ostrava and Těšín in Poland, was carried out.
- The mobility atlas at the time of the COVID-19 pandemic provided a number of indicators of population mobility within the Czech Republic, including inter-district travel; anonymised big data from the mobile network were used to extract them.
- As part of the H2020 OpenQKD project, a quantum key distribution demonstrator was developed and presented at ECOC 2021 in Bordeaux and is available at www.open-qkd.eu.
- The completion of the H2020 Tetramax 2017-2021 project, which among other things implemented technology transfer in the field of IoT.

↔ Salomon

Salomon was the second Ostrava supercomputer in history, and was at the time of its commissioning the 40th most powerful supercomputer in the world according to the TOP500 list. Over its six years of operation, it computed 8,700,000 computational tasks across 1,085 research projects.

6

Educational and Training Activities

Educational activities

IT4Innovations together with the Faculty of Electrical Engineering and Computer Science of VSB-TUO runs the **Computational Sciences PhD study programme**. Unique within the Czech Republic, this programme is focused exclusively on the use of HPC, HPDA, and AI in science and industry. At the end of the year 2021, there were 23 students studying within this as well as the eponymous all-university programme. The Computational Sciences PhD study programme is part of the **MathInHPC Doctoral School** (www.mathinhpc.cz), bringing together leading Czech workplaces focused on research in the field of HPC methods and their applications. Its students thus also have an opportunity to select dissertation topics from the joint portfolio of study courses provided by the participating institutions under joint supervision. The partner institutions include, for example, the Faculty of Mathematics and Physics of Charles University in Prague and the Institute of Mathematics of the CAS.

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

In addition, IT4Innovations is a member of an international consortium that is implementing the first pan-European Master's degree programme focused purely on High-performance computing: EUMaster4HPC. The consortium, led by the University of Luxembourg, includes universities, research and supercomputing centres, industrial partners, and other cooperating institutions. Starting from the 2022 winter semester, the Master's study programmes will be provided by 8 European universities. Participation of the Czech Republic in the pan-European EuroHPC Joint Undertaking enables Czech students to enrol for this study programme as well. Graduates will find careers in fast-growing fields such as HPC, High-performance Data Analysis, and Artificial Intelligence. This project is part of a wider EuroHPC strategy facilitating the development of key capabilities as well as education and training in the field of HPC to meet the needs of European science and industry.

Training activities

IT4Innovations supports the scientific community as well as its users by organising high-quality courses, tutorials, workshops, and other training events. The primary objective of these activities is to broadly enhance the competencies of users in terms of efficient use of the unique IT4Innovations supercomputing infrastructure. In a broader sense, IT4Innovations aims at increasing awareness and knowledge of the field of HPC nationwide among interested members of both academia and industry. The topics of courses offered by IT4Innovations are focused on computer systems and architectures, programming techniques and tools, and libraries and applications in the fields of HPC, HPDA, and AI.

In the field of Artificial Intelligence IT4Innovations has confirmed its long-standing know-how, which it aspires to pass on through its training activities. Georg Zitzlsberger from the Advanced Data Analysis and Simulations Lab has received two more NVIDIA Deep Learning Institute (DLI) instructor certificates for the Building Transformer-Based Natural Language Processing Applications and Fundamentals of Deep Learning courses in 2021. This expands IT4Innovations' portfolio of courses for developers and researchers who solve challenging problems using deep learning.

In 2021, IT4Innovations held eight training events and workshops attended by 271 participants. Four of them were held under the auspices of PRACE, as IT4Innovations has been a PRACE Training Center (PTC) since 2017, and three of them under EuroCC. They were:

- Python and scikit-learn for HPC (PTC course), 25. 2. 2021, online, 33 participants
  Introduction to MPI (PTC course), 25–27. 5. 2021, online, 28 participants
- Performance Analysis of GPU enabled HPC applications (PTC course), 15–16. 7. 2021, online, 19 participants
- Advanced MPI (PTC course), 19–21. 10. 2021, online, 24 participants
- Trainings for future cooperation of Fraunhofer and IT4Innovations, (EuroCC course), 26. 10. 2021, online, 10 participants
- Efficient multi-GPU and multi-node execution of AI applications and frameworks on the GPU nodes of Karolina supercomputer (EuroCC course), 3. 11. 2021, online, 44 participants
- Access to Karolina (EuroCC course), 11. 11. 2021, online, 53 participants
- Quantum Computing Workshop, 9. 12. 2021, online, 60 participants

PRACE Summer of HPC

Already for the 9th time, the Partnership for Advanced Computing in Europe (PRACE) allowed students to participate in a summer internship in European supercomputing centres, this time virtually. This opportunity was exploited by 66 students who were involved, together with their mentors, in 33 projects. IT4Innovations hosted two of them.

Carola Ciaramelletti, a student of condensed matter physics at the Università degli studi dell'Aquila, and Jenay Patel, who studies chemical engineering at the University of Nottingham, worked on the 'Molecular Dynamics on Quantum Computers' project under the supervision of Martin Beseda and Stanislav Paláček.

The second team of students was led by Jiří Tomčala. Lucia Absalom Bautista, who studies mathematics and statistics at the University of Seville, and Spyridon-Andreas Siskos, a computer science student at the University of Crete, worked on his project 'Quantum algorithms and their applications'.

↔ Excursions and lectures for the public

An integral part of IT4Innovations activities includes informing the general public about the activities of the centre as well as about the use of supercomputers. Excursions are organised for schools and interested parties from the public and commercial sector directly in the supercomputing centre building.

↔ Researcher's Night

The evening event, during which hundreds of scientific workplaces open their doors to the public, took place on Friday 24th September and attracted almost 600 visitors to the IT4Innovations building.

7

List of Projects

National Projects

Supercomputing Services Projects

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

Large Infrastructures for Research, Experimental Development and Innovation project

e-Infrastructure CZ (2020–2022)

→ Project ID: LM2018140
→ Principal investigator: Doc. Vít Vondrák

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

The main components of e-INFRA CZ include:

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

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

Operational Programme Research, Development and Education

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

→ Project ID: EF16_013/0001791
→ Principal investigator: Dr Branislav Jansík

→ The objective of this project is to upgrade and modernise the research infrastructure of IT4Innovations in order to at the very least maintain the existing technological level of HPC in the Czech Republic in comparison with developed, particularly European, countries. In 2018, the activities of this project were aimed at modernising the equipment and complementing the existing supercomputers with a more technologically advanced cluster similar in scope and purpose to the existing Anselm system (physically implemented in 2019 with the acquisition of the Barbora supercomputer). The Karolina supercomputer was procured in 2021, and exceeds the capacity of Salomon, the previously most powerful system of IT4Innovations.

Additional objectives of the project also include the support of high-quality research across the wider academic community in the Czech Republic, and the expansion of existing research activities at IT4Innovations in the field of modelling photonic and spin-photonic structures, design of progressive materials based on electronic structure calculations, and analysis of bioimages using HPC. In-house research is an important source of HPC expertise for IT4Innovations, which is reflected in the services the infrastructure provides to its users.

e-INFRA CZ: Modernisation (2020–2023)

→ Project ID: CZ.02.1.01/0.0/0.0/18_072/0015659
→ Principal investigator: Dr Branislav Jansík

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

Research and Development Projects

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

Operational Programme Research, Development and Education

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

→ Project ID: EF16_013/0001791
→ Principal investigator: Dr Branislav Jansík

→ The objective of the project is, among others, to extend IT4Innovations in-house research in the three following fields: 1) Modelling of photonic and spin-photonic structures, design of progressive materials based on electronic structure calculations, and bioimage analysis using HPC. 2) Use of approximations involving many-body effects (MB) in electrons, and the inclusion of temperature effects in computational methods, in particular anharmonic lattice vibration effects, and thus the possibility to study materials in near-realistic conditions, and phenomena at the mesoscale level (i.e. those including tens of thousands to millions of atoms, such as the effect of interfaces, dislocations, and other defects on material properties, as they exist in real materials and often limit their use). 3) Creation of a globally unique platform for the analysis of biological and biomedical image data using high-performance computing (HPC) infrastructure based on the open-source Fiji platform.

Artificial Intelligence and Reasoning (2017–2022)

→ Project ID: CZ.02.1.01/0. 0/0.0/15_003/0000466
→ Principal investigator: Prof. Václav Snášel

→ The Artificial Intelligence and Reasoning project yields significant measures for the development of informatics, robotics, and cybernetics research at the Czech Technical University in Prague. The project envisions the establishment of a new AI and Reasoning research group within a given part of the Czech Institute of Informatics, Robotics, and Cybernetics (CIIRC), which focuses on solving advanced interdisciplinary problems of high technical as well as social priority. The project is also supported by national partners (VSB – Technical University of Ostrava and the University of West Bohemia in Pilsen). The motivation for their participation stems from the emphasis on concentration and integration of resources, sharing of knowledge and infrastructure, and last but not least, on establishing a "unified space for opportunities" for young talent in the Czech Republic.

Modelling of Collision Processes in Low-Temperature Plasma

→ Project ID: DGS/TEAM/2020-020
→ Principal investigator: Martin Beseda

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

↔ Karolina

The fifth IT4Innovations supercomputer was commissioned in the summer of 2021 as part of the pan-European EuroHPC Joint Undertaking, which finances the acquisition of supercomputers in several European countries. Karolina is currently the most powerful supercomputer in the Czech Republic, and is one of the five EuroHPC petascale supercomputers.

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

→ Project ID: DGS/TEAM/2020-008
→ Principal investigator: Markéta Hrabánková

→ There is a high need to visualise data from large computations on High-Performance Computing (HPC) systems. It is important to monitor such systems during their runtime and visualise this information properly. To explore the data in a more intuitive way it is desirable to use 3D visualisations. For this purpose, we want to create open-source based tools that will allow us to process and visualise the data in a high quality way, and will support showcasing the data in Virtual Reality (VR). Our developed tools will specifically focus on medical data visualisation, HPC cluster runtime monitoring, and visualisation of simulation results from parallel open-source simulation tools. High quality visualisations in VR are the main goal of the project. As another goal, we want to strengthen cooperation among researchers with different specialisations. Researchers in the student grant belong to several different faculties at the university, and they will work together to fulfil the project's target. There is an aim to extend collaboration with the international partners also. Specifically, our collaboration with HLRS (HPC Center Stuttgart), with whom we already cooperate in the European project (POP), will be broadened. Similarly, our cooperation with the Blender Institute, with whom we have collaborated in the preparation of several open movies, will be extended.

The project will also enable and visualise resource consumption monitoring of IT4Innovations HPC clusters. Not only administrators and users of these systems will benefit from this feature, but it could also lead to research based on the obtained data, such as power aware job scheduling research.

Novel sources of THz radiation based on spintronic effects

→ Project ID: DGS/TEAM/2020-027
→ Principal investigator: Pierre Koleják

→ The terahertz (THz) spectral range holds immense potential for medical, security, and telecommunications applications. Therefore, it is desireable to develop new sources of terahertz waves with fast response, intense signal, controlled polarisation properties, and easy implementation. We will design, develop, and characterize THz sources exploiting spintronic phenomena such as terahertz spintronic emitters based on the spin-Hall effect and spin-laser based THz sources. Photonic and plasmonic structures will be employed to enhance the performance of these devices, including Bragg grating and plasmonic materials for spintronic emitters and anisotropic 2D grating for spin lasers. We will use non-conventional characterisation methods including terahertz plasma-based time-domain spectroscopy and pump-probe terahertz measurements to describe spin mobility and broadband optical properties. Numerical simulations of ultrafast dynamics and spin-transport will allow the deep understanding of spin based generation processes. The project is highly interdisciplinary, including approaches and methods from optics, magnetism, engineering, advanced nanotechnology, high-performance computer modelling, and applied quantum theory.

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

→ Project ID: DGS/TEAM/2020-033
→ Principal investigator: Michal Molčan

→ The latest advances in High-Performance Computing (HPC), in particular the constantly increasing available power of modern supercomputers, have enabled the creation of high-fidelity computational models and determination of their behaviour within a reasonable timeframe. Because of the scalability issues of the current computational procedures, modern scalable algorithms must be developed to utilise the full potential of HPC architectures.

The proposed project aims to develop computational procedures focusing on solving nonlinear structural dynamical problems. Moreover, the procedures will be applied to computational models of rotating machinery, discretised by three-dimensional finite elements to analyse their vibrations. Within the scope of this project, investigators will develop procedures for: 1. steady-state response determination utilising the Harmonic Balance Method (HBM), 2. determination of the amplitude-frequency response curve by the continuation technique, 3. stability and essential bifurcation analysis of the steady-state response, 4. identification of an optimal strategy for the amplitude-frequency response curve determination by application of Total Finite Element Tearing and Interconnecting (T-FETI) on a linearised model, including application of suitable preconditioners and coarse space projectors, and 5. determination of the transient response of the model, based on corotational finite element formulation utilising time-integration. The procedures will be created and studied on the test cases in MATLAB, and subsequently implemented in ESPRESO (ExaScale PaRallel FETI SOlver), developed as open source code project at IT4Innovations National Supercomputing Center and tested on real industrial cases.

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

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

→ Project ID: 8x20050
→ Principal investigator: Dr Dominik Legut

→ The research is a complementary joint work of the following institutions: VSB – the Technical University of Ostrava, Prešov University, and the Donau-University Krems of the Czech Republic, Slovakia, and Austria, respectively. The project consists of finding novel RE-free permanent magnets by means of a detailed systematic study of Fe-Ta and Fe-Hf compounds using adaptive genetic algorithms. Best predicted structures, i.e. those exhibiting negative enthalpy (an indication of phase stability), high saturation magnetisation, and a uniaxial lattice are further tested to see if they also exhibit high magnetocrystalline anisotropy, exchange integrals (J's), and temperature (Tc) of transition from magnetic to paramagnetic state. First, MAE and J's will be obtained from the quantum mechanical calculations using HPC infrastructure, followed by Tc obtained from the atomic spin dynamic calculations. The structural parameters of the most stable candidates will then be transferred to the Slovak partners to synthesise samples and to measure the number of magnetic quantities like magnetisation, magnetic susceptibility etc. At the same time the Austrian partner will perform micromagnetic simulations to determine the magnetic behaviour of given materials with respect to their texture, shape, and thickness, under various thermal conditions.

Projects supported by the Moravian-Silesian Region

Individual projects

Digital Innovation Hub – Pilot Verification (2020–2022)

→ Project ID: 08183 2019 RRC (S516/20-96100-01RN)
→ Principal investigator: Martin Duda

→ Financial support from the Moravian-Silesian Region for the provision of discounted services related to the use of the computing capacity of IT4Innovations National Supercomputing Center. This support is intended for small and medium-sized enterprises with a registered office or branch in the Moravian-Silesian Region and is provided under a de minimis regime for the period 2020-2022. The aim of this support is to enable progressive small and medium-sized enterprises, including start-ups, to use supercomputing (HPC) technologies and expertise for the development of their business.

Science and Research projects in the Moravian-Silesian Region

Projects of talented VSB-TUO PhD students

→ Project ID: 07685/2019/RRC
→ Principal investigator: Prof. Tomáš Kozubek

→ The aim of this project is to support talented PhD students at VSB-TUO. The support of students will be in the form of the payment of an additional contribution to the regular doctoral scholarship for students. VSB-TUO in cooperation with the Moravian-Silesian Region wants to contribute to better conditions for students in their scientific activities, especially in relation to the use of the results of their scientific work in the application sphere.

Projects supported by the Grant Agency of the Czech Republic

International grant projects evaluated by the LEAD Agency

Space-time Boundary Element Methods for the Heat Equation (2019–2021)

→ Project ID: 19-29698L
→ Principal investigator: Dr Michal Merta

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

Standard grant projects

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

→ Project ID: 20-18392S
→ Principal investigator: Dr Andrzej Kądzielawa

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

Projects supported by the Technology Agency of the Czech Republic

National Centres of Competence Programme

Personalised Medicine – Diagnostics and Therapy (2019–2022)

→ Project ID: TN01000013
→ Principal investigator: Dr Jan Martinovič

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

TREND Programme

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

→ Project ID: FW2020151
→ Principal investigator: Dr Kateřina Slaninová

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

→ The main objective will be achieved through the development and subsequent clinical testing of the software prototype of an expert system for the automatic evaluation of pathologies from eye images in the diagnosis of diabetic retinopathy. The expert system will use a computer neural network and mathematical and statistical meth-

ods to demonstrate its ability to automatically evaluate pathologies on eye images at a similar quality to fully qualified medical staff, and this ability will then be clinically validated on real data.

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

→ Project ID: FW01010274
→ Principal investigator: Dr Petr Strakoš

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

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

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

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

Projects supported by the Ministry of Industry and Trade

TRIO Programme projects

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

→ Project ID: FV30104
→ Principal investigator: Dr Tomáš Brzobohatý

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

Projects of Operational Programme Enterprise and Innovation for Competitiveness

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

→ Project ID: CZ.01.1.02/0.0/0.0/17_176/0015651
→ Principal investigator: Dr Tomáš Brzobohatý

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

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

→ Project ID: CZ.01.1.02/0.0/0.0/20_321/0024896
→ Principal investigator: Dr Kateřina Slaninová

→ The project goal is to create a SmartFleet platform which should enable optimisation of company car fleets in terms of their composition and utilisation, with the aim to maximise the share of cars that use alternative fuels (especially electric cars). The solution will be developed as interdisciplinary and open, which allows flexibility in terms of new inputs (e.g. location of hydrogen stations in the future) and enables iteration when considering modification of the car fleet and solving complete car fleet lifecycles – from purchase planning and daily planning to online monitoring and response to everyday changes.

Holograms with active safety elements (2021–2023)

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

→ The aim of the joint industrial research project of Optaglio a.s. and VSB – Technical University of Ostrava is to develop new products in the field of security holography that will be competitive on global markets. These are completely new types of anti-counterfeiting features. In the framework of the presented project we will focus on two original approaches to security holography, combining a high technical level of production and advanced methods of nanostructure design.

Educational Projects

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

Projects of Operational Programme Research, Development and Education

Doctoral School for Education in Mathematical Methods and Tools in HPC (2017–2022)

→ Project ID: CZ.02.2.69/0.0/0.0/16_018/0002713
→ Principal investigator: Prof. René Kalus

→ The main objective of the project is to establish the Doctoral School for Education in Mathematical Methods and Tools in HPC, integrating doctoral studies at Charles University, the Czech Academy of Sciences, and VSB-TUO. Part of the project is to modernise and internationalise one of the doctoral programmes of the school (Computational Sciences, VSB-TUO) as well as to create new double-degree programmes (planned in collaboration with Università della Svizzera italiana, Lugano, Switzerland, and l'Université Toulouse III Paul Sabatier, France). → www.mathinhpc.cz

Technology for the Future 2.0 (2019–2022)

→ Project ID: CZ.02.2.69/0.0/0.0/18_058/0010212
→ Principal investigator: Prof. René Kalus

→ The project aims at enhancing the quality and profile of educational activities and increasing their relevance for the labour market. It implements new forms of educational methods, establishes new study programmes, and boosts the internationalisation of

↔ LUMI

In addition to the supercomputers operated by IT4Innovations, the Czech research community is also using the computational resources of the LUMI supercomputer, which has been installed in Kajaani, Finland, since the end of 2021. Thanks to IT4Innovations' membership in the LUMI consortium, which consists of ten European countries, Czech scientists will have access to one of the world's most powerful and advanced supercomputers, the peak theoretical performance of which is expected to exceed 550 PFlop/s in 2022.

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

Science without Borders 2.0 (2020–2023)

→ Project ID: CZ.02.2.69/0.0/0.0/18_053/0016985
→ Principal investigator: Prof. Tomáš Kozubek

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

VSB-TUO projects with IT4Innovations participation

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

→ Project ID: VI20192022169
→ Principal investigator: Petr Berglowiec (Faculty of Electrical Engineering and Computer Science, VSB-TUO)
→ Grant Provider: Ministry of the Interior of the Czech Republic

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

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

→ Project ID: TJ02000157
→ Principal investigator: Jan Vysocký (ENET Centre, VSB-TUO)
→ Grant Provider: Technology Agency of the Czech Republic

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

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

→ Project ID: TJ02000031
→ Principal investigator: Dr Jan Fulneček (ENET Centre, VSB-TUO)
→ Grant Provider: Technology Agency of the Czech Republic

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

National Centre for Energy (NCE) (2019–2022)

→ Project ID: TN01000007
→ Principal investigator: Prof. Stanislav Mišák (ENET Centre, VSB-TUO)
→ Grant Provider: Technology Agency of the Czech Republic

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

Energy system for grids (2019–2023)

→ Project ID: TK02030039
→ Principal investigator: Prof. Stanislav Mišák (ENET Centre, VSB-TUO)
→ Grant Provider: Technology Agency of the Czech Repulic

→ The aim of the project is the development of a new system solution for energy flow control in the energy platform of a Sophisticated Energy System (SEN) on the level of distribution networks to supply energy platforms of municipalities, towns, and microregions. The SEN will be supported by sophisticated control methods and prospective technologies to increase its security, reliability, raw material self-reliance, and energy self-sufficiency, while maximising the exploitation of decentralised, particularly renewable sources of energy. The objective is to ensure the readiness for a change in the energy system control concept after implementing the EU Winter Package, in compliance with the National Action Plan for Smart Grids and the updated State Energy Conception within the 5-year implementation of the project.
→ Project ID: TK03020027

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

→ Principal investigator: Prof. Stanislav Mišák (ENET Centre, VSB-TUO)
→ Grant Provider: Technology Agency of the Czech Republic

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

International Projects

Supercomputing Services Projects

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

PRACE-6IP – Partnership for Advanced Computing in Europe, 6th Implementation Phase (2019–2022)

→ Project ID: 823767 (Call H2020 INFRAEDI-2018-2020)
→ Principal investigator: Doc. Vít Vondrák

→ The objective of the project is to build on the previous successful PRACE projects, the task of which was to implement the European HPC infrastructure and to continue to develop supercomputing cooperation to strengthen the competitiveness of European science, research, and industry. Unlike the previous ones, already the sixth project in a row to support the pan-European PRACE research infrastructure and its users is focused on the identification and development of new applications with significant potential to exploit the capacity of exascale supercomputers. → www.prace-ri.eu

Research and development projects

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

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

→ Project ID: 951732 (H2020-JTI-EuroHPC-2019-2)
→ Principal investigator: Dr Tomáš Karásek

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

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

→ Project ID: ID 825532 (H2020-ICT-2018-2020)
→ Principal investigator: Dr Jan Martinovič

→ The objective of this project, for which IT4Innovations was the coordinator, was to develop an engineering platform using state-of-the-art technologies such as

high-performance computing, big data, and cloud services. The benefits coming out of the LEXIS project were demonstrated via three pilot tests suitable for industrial fields, including aerospace, weather and climate, and earthquakes and tsunami.
→ www.lexis-project.eu

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

→ Project ID: 824080 (H2020-INFRAEDI-2018-1)
→ Principal investigator: Dr Lubomír Říha

→ The POP2 Centre of Excellence in HPC builds on the Performance Optimisation and Productivity 1 (POP1) project and extends its activities. The main aim of POP2 is to assist with the analysis of parallel applications, identify erroneous parts of codes, and make recommendations of optimisation methods resulting in increased performance and better scalability of a given application. → www.pop-coe.eu

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

→ Project ID: 956137 (H2020-JTI-EuroHPC-2019-1, EuroHPC-IA)
→ Principal investigator: Dr Jan Martinovič

→ The project LIGATE aims to integrate and co-design best in class European open-source components together with proprietary IPs to keep worldwide leadership on Computer-Aided Drug Design (CADD) solutions exploiting today's high-end supercomputers and tomorrow's Exascale resources, fostering European competitiveness in this field. The proposed LIGATE solution, in a fully integrated workflow, enables the delivery of the result of a drug design campaign with the highest possible speed and accuracy; further, implementing the auto-tuning of the parameters of the solutions helps to meet the time and resource constraints. → www.ligateproject.eu

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

→ Project ID: 957269 (H2020-ICT-2018-20 / H2020-ICT-2020-1)
→ Principal investigator: Dr Kateřina Slaninová

→ The project aims to develop a holistic approach for co-designing computation and communication in a state-of-the-art and, primarily, secure system for HPDA. This is achieved by simplifying the programmability of heterogeneous and distributed architectures through a "data-driven" design approach, the use of hardware-accelerated AI, and through efficient monitoring of the execution with a unified hardware-software paradigm. The project will validate its approach through three case studies, a weather-based prediction model, an air quality monitoring application, and a traffic modelling framework for smart cities. → www.everest-h2020.eu

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 ACROSS project will co-design and develop an HPC, BD, and Artificial Intelligence (AI) convergent platform, supporting applications in the aeronautics, climate and weather, and energy domains. To this end, ACROSS will leverage the next generation of pre-exascale infrastructures, still being ready for exascale systems, and also leverage effective mechanisms to easily describe and manage complex workflows in the three aforementioned domains. ACROSS will combine traditional HPC techniques with AI (specifically machine learning/deep learning) and BD analytic techniques to enhance the application test case outcomes. → www.acrossproject.eu

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

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

→ s-NEBULA explores and develops a revolutionary approach to teraHertz (THz) technology, both for the generation and detection of THz radiation, initiating the new field of spin-based teraHertz technology, a game changer for the future of THz field. The ambition of the project is to provide a platform of room-temperature innovative spin-based THz building blocks, arising from novel combinations of magnetism and optics. s-NEBULA will provide cutting-edge solutions to solve bottleneck scientific issues in the THz field, motivated by clear needs in judiciously chosen target applications. → www.s-nebula.eu

SCALABLE – SCAlable LAttice Boltzmann Leaps to Exascale (2021–2023)

→ Project ID: 956000 (H2020-JTI-EuroHPC-2019-1, EuroHPC-IA)
→ Principal investigator: Dr Lubomír Říha

→ In the SCALABLE project, eminent industrial and academic partners team up to improve the performance, scalability, and energy efficiency of an industrial Lattice Boltzmann methods-based computational fluid dynamics (CFD) software. Lattice Boltzmann methods (LBM) have already evolved to become trustworthy alternatives to conventional CFD. LBM is especially well suited to exploit advanced supercomputer architectures through vectorisation, accelerators, and massive parallelisation. The project will directly benefit European industry, while contributing to fundamental research. → www.scalable-hpc.eu

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

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

→ IO-SEA aims to provide a novel data management and storage platform for exascale computing based on hierarchical storage management (HSM) and on-demand provisioning of storage services. The platform will efficiently make use of storage tiers spanning NVMe and NVRAM at the top all the way down to tape-based technologies. Advanced IO instrumentation and monitoring features will be developed in the IO-SEA project leveraging the latest advancements in AI and machine learning to systematically analyse the telemetry records to make smart decisions about data placement. → www.iosea-project.eu

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

→ Project ID: 800898 (H2020-FETHPC-2016-2017)
→ Principal investigators: Dr Tomáš Karásek and Dr Jan Martinovič

→ The objective of ExaQUte, a three-year project, was to develop new methods that allow the solution of complex engineering problems using numerical simulations on future exascale systems. Within the project, new computing methods and software tools were developed for solving simulations of aerodynamics for optimising geometrically complex civil engineering structures. IT4Innovations participated in deploying the Hyperloom and COMPSs tools using high-performance computing systems, their

configuration, and optimisation. Our participation also included testing of robust algorithms for shape optimisation of wind-loaded structures. → www.exaqute.eu

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

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

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

CloudiFacturing – Cloudification of Production Engineering for Predictive Digital Manufacturing (2017–2021)

→ Project ID: 768892 (Call no. H2020-FOF-2017)
→ Principal investigator: Dr Tomáš Karásek

→ The mission of the project was to contribute to efficient use of high-performance computing by European small and medium-sized manufacturing companies, and thus increase their competitiveness. This project aimed at optimisation of production processes and productivity of companies through using HPC-based modelling and simulation as cloud services. → www.cloudifacturing.eu

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

→ Project ID: 761349 (Call no. H2020-ICT-2016-2)
→ Principal investigator: Prof. Miroslav Vozňák

→ Within this project, the "Smart Anything Everywhere" initiative was implemented in the field of customised low energy computing for cyberphysical systems and the Internet of Things. The key purpose of this initiative was to accelerate innovations in European industry. The initiative connected technical and application knowledge and experience, which helped small and medium-sized enterprises adopt advanced digital technologies more effectively and efficiently. → www.tetramax.eu

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

→ Project ID: 721865
→ Principal investigator: Prof. Tomáš Kozubek

→ The objective of the project was to educate researchers able to participate in interdisciplinary cooperation. The collaboration between industrial partners and research organisations speeded up the development of key technologies for the development of turbines and hasten their implementation in practice. → www.msca-expertise.eu

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

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

→ The DICE consortium brings together a network of computing and data centres, research infrastructures, and data repositories for the purpose of enabling a European storage and data management infrastructure for EOSC, thereby providing generic services and building blocks to store, find, access and process data in a consistent and persistent way. → www.dice-eosc.eu

Educational Projects

Erasmus+ projects

SCtrain – Supercomputing knowledge partnership (2020–2023)

→ Project ID: 20-203-075975 (KA203-6E6A1FFC)
→ Principal investigator: Prof. Tomáš Kozubek

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

List of Abbreviations

AI	Artificial Intelligence
ACROSS	HPC big dAta artifiCial intelligence cross stack platfoRm tOwardS exaScale
BD	Big Data
BDVA/DAIRO	Big Data Value Association/Data, AI and Robotics
CEET	Centre for Energy and Environmental Technologies
CloudiFacturing	Cloudification of Production Engineering for Predictive Digital Manufacturing
CR	Czech Republic
CT	Computed Tomografy
DICE	Data Infrastructure Capacity for EOSC
DIH	Digital Innovation Hub
DIHnet EU	Digital Innovation Hub Networks
DOI	Digital Object Identifier
DS	Distribution system
ECOC	European Conference on Optical Communication
EOSC	European Open Science Cloud
ESA	European Space Agency
ETP4HPC	European Technology Platform for High-Performance Computing
EUDAT CDI	EUDAT Collaborative Data Infrastructure
EUMaster4HPC	European Master For High Performance Computing
EUROCC	National Competence Centres in the framework of EuroHPC
EuroHPC JU	The European High Performance Computing Joint Undertaking
EVEREST	dEsign enVironmEnt foR Extreme-Scale big data analyTics on heterogeneous platforms
ExaQUte	Exascale Quantifications of Uncertainties for Technology and Science Simulation
EXPERTISE	Experiments and High-Performance Computing for Turbine Mechanical Integrity and Structural Dynamics in Europe
FP7	Seventh Framework Programme
FTE	Full-time equivalent
GA CR	Grant Agency of the Czech Republic
GPU	Graphics Processing Unit
H2020	Horizon 2020
HPC	High-Performance Computing
HPDA	High Performance Data Analytics
HW	Hardware
I4MS	ICT Innovation for Manufacturing SMEs
ICT	Information and communications technology
IF	Impact Factor
IO-SEA	IO Software for Exascale Architecture
IoT	Internet of Things
IRS	Integrated Rescue System
LEXIS	Large-scale Execution for Industry & Society
LIGATE	LIgand Generator and portable drug discovery platform AT Exascale
LUMI	Large Unified Modern Infrastructure
MEYS CR	Ministry of Education, Youth and Sports of the Czech Republic
MPI	Message Passing Interface
MSR	Moravian-Silesian Region
NCE	National Centre for Energy
NVIDIA DLI	NVIDIA Deep Learning Institute
OAGC	Open Access Grant Competitions
OPENQKD	Open European Quantum Key Distribution Testbed
POP2	Performance Optimisation and Productivity 2
PRACE	Partnership for Advanced Computing in Europe
PRACE-6IP	Partnership for Advanced Computing in Europe, 6th Implementation Phase
PTC	PRACE Training Center
QKD	Quantum Key Distribution
R&D&I	Research, Development and Innovation
SCALABLE	SCAlable LAttice Boltzmann Leaps to Exascale
SCtrain	Supercomputing knowledge partnership
SMEs	Small and medium-sized enterprises
s-NEBULA	Novel Spin-Based Building Blocks for Advanced TeraHertz Applications
SW	Software
TA CR	Technology Agency of the Czech Republic
TETRAMAX	Technology Transfer via Multinational Application Experiments
VR	Virtual Reality
VSB-TUO	VSB — Technical University of Ostrava

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

www.it4i.eu

Postal address:
VSB — Technical University of Ostrava
17. listopadu 2172/15
708 00 Ostrava
Czech Republic

E-mail info@it4i.cz
Phone. +420 597 329 500

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

This publication was supported by The Ministry of Education, Youth and Sports from the Large Infrastructures for Research, Experimental Development and Innovations project "e-Infrastructure CZ" (LM2018140).

MINISTRY OF EDUCATION, YOUTH AND SPORTS