VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

REVIEW 2019

REVIEW 2019

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Managing Director‘s Introduction

Dear Readers,

It is no exaggeration to say that the year 2019 will surely rank among those very significant and successful years in our centre‘s history. Success was achieved in the field of research, supercomputing infrastructure development, cooperation with industry, and education, all of which are the main pillars of our activity. I am particularly pleased to share our achievements with you on the pages of our 2019 Review.

Every supercomputing centre‘s source of pride is its supercomputing systems. At IT4Innovations, two new systems were procured in 2019, extending the total number from two to four after five years. The first one, which was installed in the spring, is NVIDIA DGX-2, a very powerful system specialized for artificial intelligence calculations using powerful GPUs. In the autumn, the long-awaited modernization of our first Anselm supercomputer was performed by installing Barbora, a state-of-the-art supercomputer. With its theoretical peak performance of 849 TFlop/s, it ranked second in our internal performance ranking. So we already have these systems. However, we also achieved significant success in building supercomputing infrastructures against international competition. In the pan-European competition to host EuroHPC petascale systems, which was announced by the EuroHPC Joint Undertaking, we were successful with our project titled IT4Innovations Centre for European Science and Industry, which bears the working title EURO_IT4I. This system will allow both Czech and international scientists as well as industrial partners to obtain access to the state-of-the-art world-class supercomputer. Its theoretical peak performance will range around 13 PFlop/s, ranking it 10th in Europe and no lower than 50th worldwide. What is more, we also became a member of the LUMI (Large Unified Modern Infrastructure) consortium bringing together 10 European countries to procure as well as operate, together with the European Commission, practically the most powerful European supercomputer, the EuroHPC pre-exascale system. The LUMI supercomputer, which is to be located in Kajaani in Finland, and will rank among the world‘s top ten, will thus be made available to Czech scientists and industry.

IT4Innovations has established strong, long-term international connections and is currently involved in a number of prestigious, international organizations, infrastructures, and initiatives such as PRACE, ETP4HPC, and EuroHPC JU. Last year, we extended our portfolio of memberships to other important European organizations, namely BDVA (the Big Data Value Association) and EUDAT CDI (Collaborative Data Infrastructure).

However, supercomputers themselves without projects using their computational resources to achieve their goals would serve no purpose. We are proud not only of the tens of national projects but also, and primarily, of international projects funded mainly by the EU Horizon 2020 programme. At the beginning of 2019 we started to implement LEXIS, currently our most important project, which brings together 16 members across Europe, and the objective of which is to develop an advanced engineering platform for solving complex engineering problems using state-of-the-art technologies such as high-performance computing, big data, and cloud services. It is the very first project of such importance coordinated by VSB – Technical University of Ostrava. Achievements in research and development worth mentioning also include the publication activities of our colleagues; several of them have achieved success in leading international journals. We also received several best poster awards and presented our research at prestigious international conferences, which I am particularly pleased about.

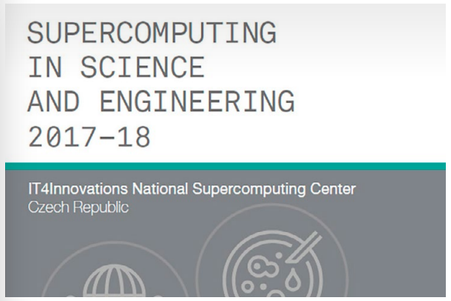
We reinforced our connections in the field of cooperation with industrial enterprises, primarily in developing activities within the Digital Innovation Hub. Our activities last year were aimed at establishing the Digital Innovation Hub Ostrava in cooperation with the Moravian-Silesian Innovation Centre (MSIC). The strategic objective of the DIH Ostrava is to support implementation and use of advanced digital innovations in industry and society alike. We have great potential to become one of the European Digital Innovation Hubs.

I am proud of the fact that IT4Innovations can be considered a leading HPC research centre of pan-European extent, as well as it providing its users and partners with a wider portfolio of services and a more generous amount of computational resources. I would particularly like to thank our employees, partners, and supporters, without whom we would not otherwise be able to achieve the above-mentioned particular examples of success, which are presented in more detail on the following pages of this publication.

Vít Vondrák

Managing Director of IT4Innovations
National Supercomputing Center

IMPORTANT EVENTS IN 2019



JANUARY

- Commencement of the **LEXIS** project, for which IT4Innovations is the Coordinator. It is the very first Horizon 2020 project coordinated by VSB-TUO. The objective of the project is to develop an advanced engineering platform using state-of-the-art technologies such as high-performance computing, big data, and cloud services.
- Hosting of the **FIJI Hackathon** focused on parallelization and HPC. For the first time, it took place in the Czech Republic.
- Registration of IT4Innovations by the European Commission as a **Digital Innovation Hub** for cooperation with industry in the field of HPC and advanced data analysis.
- Successful fulfillment of the **ANTAREX** project objectives.
- Participation of IT4Innovations together with the ENET Centre in the **National Centre for Energy** (NCE).

FEBRUARY

- Successful completion of the **ExCAPE** project, which was aimed at developing computer programs capable of finding new drugs using exascale computer systems.
- **Euronews** shot a report at IT4I, broadcasted as part of the Smart Regions program, which reports on important projects with high added value for European Union citizens.

MARCH

- Launching of the **NVIDIA DGX-2** system specialized for artificial intelligence calculations. It is the very first installation of this type in Central and Eastern Europe.
- Membership obtained in the **Big Data Value Association** (BDVA), an international non-profit organization.
- The Digital Revolution seminar organized by the **CzechInno** association took place at IT4Innovations.
- Participation at **Kariéra PLUS**, a job fair organized by VSB – Technical University of Ostrava.
- Meeting of the partners of the **InnoHPC** project (High-Performance Computing for Effective Innovation in the Danube Region) held at IT4Innovations.

APRIL

- Publication of the **Supercomputing in Science and Engineering 2017–18** proceedings, which includes 51 contributions from our infrastructure users.
- Accession to the **EUDAT Collaborative Data Infrastructure**. It is a European e-infrastructure integrating data services and resources to boost research.

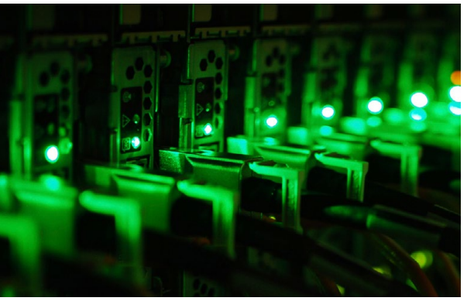
MAY

- Organization of the **High-Performance Computing in Science and Engineering** (HPCSE) conference.
- New membership in a research consortium in the field of personalized medicine – the **PerMed National Centre of Competence**.
- **The Best PRACEdays19 Poster** Award received by our colleague Martin Golasowski for his contribution entitled Distributed Environment for Traffic Simulations.
- Official launching of the **6th Implementation Phase of the PRACE** (Partnership for Advanced Computing in Europe) project.
- The meeting of the Selection Committee of the **Joseph Fourier Prize Competition** held at IT4Innovations.

JUNE

- Success achieved in the pan-European competition to host the **EuroHPC petascale supercomputer**, which will be built within the implementation of the EuroHPC Joint Undertaking. With its parameters, this supercomputing system will rank among the most powerful supercomputers in Europe. Simultaneously, IT4Innovations achieved success in the competition to build a EuroHPC pre-exascale supercomputing system as a member of the **LUMI** (Large Unified Modern Infrastructure) consortium formed by Finland as the Coordinator, and Belgium, Denmark, Estonia, the Netherlands, Norway, Poland, Sweden, and Switzerland. By the end of the year 2020, the system will have been installed in Kajaani, Finland, and will become one of the most powerful systems in Europe, as well as worldwide. The official announcement about the hosting was made on 13th June 2019 with the participation of Khalil Rouhana, the Deputy Director-General of the European Commission for Communication networks, Content, and Technology.
- Our colleague Tomáš Martinovič presented a research project entitled HPC Oriented Algorithm for Computation of Recurrence Quantitative Analysis which won the **Best Poster Award at the ISC 2019 conference**.

IMPORTANT EVENTS IN 2019



JULY

> Together with other two research infrastructures – the CESNET association and CERIT-SC centre operated by Masaryk University, we implemented the **e-INFRA** CZ project. e-INFRA CZ is 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.

AUGUST

> Already for the seventh time, we were involved in the **PRACE Summer of HPC** program and hosted two foreign students as part of their summer internship. The program is designed for students from European universities and is focused on HPC projects in supercomputing centers integrated in the Partnership for Advanced Computing in Europe (PRACE) project.

> Celebration of the 5th anniversary of the **IT4Innovations building completion**.

SEPTEMBER

> Launching of another HORIZON 2020 project – **OPENQKD**, during which implementation and testing of a pilot quantum communication infrastructure will be carried out in several European countries.

> Pavel Moravec from the Advanced Data and Simulation Lab won the **Best Paper** Award at the **CISIM 2019** conference in Belgrade, Serbia.

> Participation at the **Art&Science** festival and the **NATO Days** as well as organization of the **Researcher's Night** at IT4Innovations with more than 700 visitors.

OCTOBER

> Opening ceremony for the launch of our new supercomputer, which was named **Barbora**.

> Launching of the **Doctoral School** for Education in Mathematical Methods and Tools in HPC.

> Barbora Kacerovská from the Modelling for Nanotechnologies Lab was announced the winner of the Lady Business competition in the **Exceptional Student of the Moravian-Silesian Region** category.

> Organization of the **Czech-French workshop** focused on nanotechnologies.

> Co-organization of the **DS-RT conference** (Distributed Simulation and Real Time Applications) held in Cosenza, Italy.

NOVEMBER

> In Strasbourg, the EuroHPC pre-exascale and petascale systems **hosting agreements were signed.**

> The **3rd IT4Innovations Users Conference and the 8th Annual Conference of IT4Innovations Centre of Excellence** were held.

> The IT4Innovations **Digital Innovation Hub** was awarded the best DIH of November by DIHnet EU.

> IT4Innovations was among the exhibitors at the **Supercomputing Conference** (SC19) in Denver, USA. At the conference, two articles by Jakub Beránek dealing with network-accelerated non-contiguous memory transfers and interface design for FPGA communication were published. On the occasion of its 20th edition, the presentation of the **HyperLoom** project poster was selected for the SC History exhibition.

DECEMBER

> The research team led by Prof. Zelinka at VSB-TUO and colleagues from the Big Data Lab received an honorary award from the expert panel within the **Visionaries 2019** project competition for their Chiméra mobile application for encrypted communication.

IT4INNOVATIONS PROFILE

IT4Innovations National Supercomputing Center at VSB – Technical University of Ostrava (hereafter referred to as IT4Innovations) represents a strategic large research infrastructure in the Czech Republic, and together with other two infrastructures, CESNET and CERIT-SC, constitutes e-INFRA, the E-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.

IT4Innovations provides state-of-the--art supercomputing technologies and services to both Czech and international research teams from academia and industry. At present, IT4Innovations runs four supercomputers – Anselm (94 TFlop/s, installed in the summer of 2013), Salomon (2 PFlop/s, installed in the summer of 2015), Barbora (849 TFlop/s, installed in the autumn of 2019) and the NVIDIA DGX-2 system specialized for artificial intelligence calculations (130 TFlop/s and 2 PFlop/s in AI, installed in the spring of 2019).

IT4Innovations conducts excellent research in the field of High-Performance Computing (HPC), High Performance Data Analysis (HDPA), and Artificial Intelligence (AI). The main research areas of IT4Innovations include big data processing and analysis, machine learning, development of parallel scalable algorithms, solution of complex engineering problems, advanced visualization, virtual reality, modelling for nanotechnologies, and material design.

IT4Innovations research activities are executed across five laboratories:

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

IT4Innovations also has a strong focus on cooperation with industrial enterprises, earning IT4Innovation the status of “Digital Innovation Hub”, registered at the European Commission level, and is a member of DIHnet EU, the European network of digital innovation hubs. Digital innovation hubs are based on regional cooperation among a diversity of partners such as research organizations, industrial associations, incubators/accelerators, and particular companies. In this context, IT4Innovations has developed a partnership with the Moravian-Silesian Innovation Center Ostrava.

IT4Innovations is focused not only on providing access to state-of-the-art supercomputing systems and on activities in science and research, but also on offering 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 Science PhD study program. This program is jointly guaranteed by IT4Innovations and the Faculty of Electrical Engineering and Computer Science at VSB-TUO. In addition, the center’s employees participate in providing education in computationally-based study programs offered by VSB-TUO on all levels ranging from BSc to PhD study programs such as computational and applied mathematics, nanotechnology, applied mechanics, and applied physics.

History

2011

- The foundation of IT4Innovations
- Became a Member of 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

- Became a Member of ETP4HPC (European Technology Platform in the area of High-Performance Computing)

2018

- The Czech Republic joined the EuroHPC JU (support for building a European exascale supercomputer), actively participating in EuroHPC activities

2019

- Launching of the NVIDIA DGX-2 system specialized for Artificial Intelligence calculation
- Launching of the Barbora supercomputer
- Decision made to install a petascale supercomputer entitled EURO_IT4I with a theoretical peak performance of about 13.6 PFlop/s in 2020
- Success achieved in the competition to build a EuroHPC pre-exascale supercomputing system as a member of the LUMI (Large Unified Modern Infrastructure) consortium
- Became a member of BDVA (Big Data Value Association) and EUDAT CDI

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, mediating its effective use in order to increase the competitiveness and innovation of Czech science and industry.

Vision

Our vision is to become a leading supercomputing center 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.

Membership

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:

PRACE
Partnership for Advanced Computing in Europe

ETP4HPC
European Technology Platform for High-Performance Computing

I4MS
ICT Innovation for Manufacturing SMEs

EUDAT
Collaborative Data Infrastructure

BDVA
Big Data Value Association

EuroHPC Joint Undertaking

ORGANIZATIONAL STRUCTURE

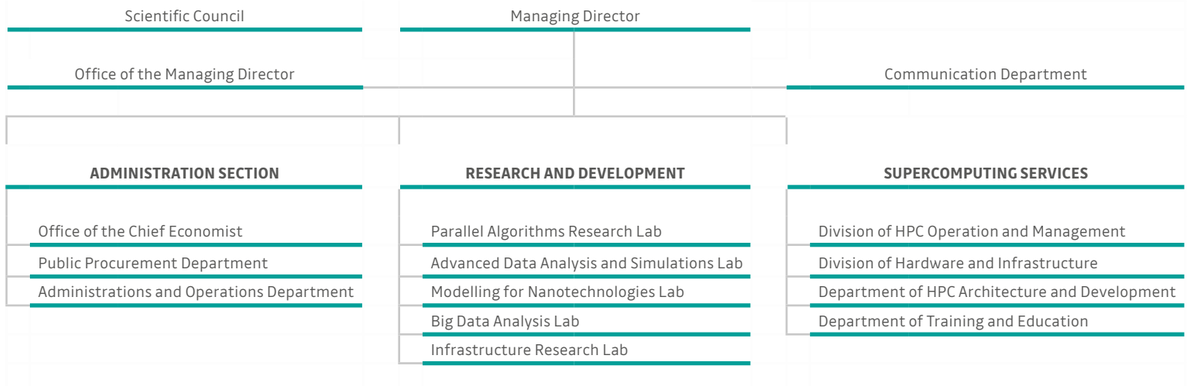
Management of IT4Innovations

Vít Vondrák
Managing Director

Radim Mrázek
Administration and Finance

Branislav Jansík
Supercomputing Services

Tomáš Kozubek
Research and Development



Management of IT4Innovations Laboratories

Dr Tomáš Karásek
Parallel Algorithms Research Lab

Dr Jan Martinovič
Advanced Data Analysis and Simulation Lab

Prof. Jaromír Pištora
Modeling for Nanotechnologies Lab

Prof. Miroslav Vozňák
Big Data Analysis Lab

Dr Lubomír Říha
Infrastructure Research Lab

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. Jaromír Pištora
Prof. Miroslav Vozňák

External

Prof. Jan Holub
Faculty of Information Technology
Czech Technical University in Prague

Doc. Jiří Jaroš
Faculty of Information Technology
Brno University of Technology

Prof. Pavel Tvrdík
Faculty of Information Technology
Czech Technical University in Prague

Doc. Stanislav Hledík
Faculty of Philosophy and Science
Silesian University in Opava

Prof. Jaroslav Pokorný
Faculty of Mathematics and Physics
Charles University

Also in 2019, IT4Innovations continued in its collaboration with the partners of the IT4Innovations Centre of Excellence project – namely the University of Ostrava, the Silesian University in Opava, Brno University of Technology, and the Institute of Geonics of the Czech Academy of Sciences. Since 2016, we have been jointly implementing the IT4Innovations Excellence in Science project, which is funded by the National Programme of Sustainability II. Supervision of this project as well as the sustainability of the original Centre of Excellence project is ensured by the Supervisory Board.

Supervisory Board Centre of Excellence IT4Innovations

CHAIRMAN

Evžen Tošenovský, Dr.h.c.

VICE-CHAIRMAN

Doc. Pavel Drozd

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Prof. Ivo Vondrák
Prof. Petr Noskievič
Miroslav Murin, FCCA
Prof. Pavel Zemčík
Leoš Dvořák
Doc. Pavel Tuleja
Prof. Miroslav Tůma

Research Infrastructure Advisory Board of IT4Innovations National Supercomputing Center / Research Council of IT4Innovations Centre of Excellence

CHAIRMAN

Doc. Vít Vondrák

MEMBERS

Prof. Jean Christopher Desplat
Irish Centre for High-End Computing

Prof. Petr Berka
University of Economics, Prague

Doc. Petr Cintula
Institute of Computer Science
The Czech Academy of Sciences

Prof. Dr. Kenneth Ruud
The Arctic University of Norway

Prof. Roman Wyrzykowski
Czestochowa University of Technology

Prof. Arndt Bode
Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences

Prof. Vahtang Jandieri
University of Duisburg-Essen

Prof. Svetozar Dimitrov Margenov
Bulgarian Academy of Sciences

Employees of IT4Innovations

Employees of IT4Innovations by divisions in full time equivalent (FTE), 135.78 FTE in total:

9% Supercomputing Services

21% Management and Administration

70% Research and Development

24% Parallel Algorithms Research Lab
38% Advanced Data Analysis and Simulation Lab
17% Modeling for Nanotechnologies Lab
9% Big Data Analysis Lab
12% Infrastructure Research Lab

FINANCIAL REVIEW

Sources of Funding

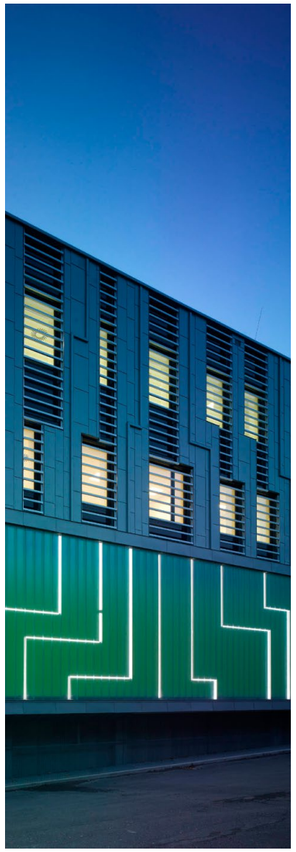
In 2019, the overall budget of IT4Innovations was CZK 315,603,000. The largest share of the funding sources for operational expenses of the institute was contributed by national grants (grants of the Ministry of Education, Youth and Sports, Technology Agency of the Czech Republic, Grant Agency of the Czech Republic, the Ministry of Industry and Trade, and the Ministry of Interior). Other funding sources for operational expenses included structural funds, internal resources, international grants, research organization development funds, contract research together with rental of computational resources, specific research, and other sources of funding.

43.3%	National grants
31.6%	Structural funds
9.2%	Internal resources
7.6%	International grants
4.6%	Research organization development funds
1.9%	Contract research and rental of computational resources
0.9%	Specific research
0.9%	Other

38.6%	LEXIS
12.6%	POP2
12.2%	PRACE 6IP
9.5%	ExaQUte
6.4%	Expertise
5.8%	PRACE 3IP
4.5%	Cloudifacturing
3.2%	PRACE 5IP
2.6%	InnoHPC
2.3%	Superheroes4Science
1.4%	TETRAMAX
0.5%	OPENQKD
0.2%	READEX
0.2%	ANTAREX

71.7%	Large Research Infrastructures for R&D&I projects – MEYS
20.7%	National Programme of Sustainability II – MEYS
3.8%	Centres of Competence – TA CR
1.4%	TRIO – MIT
0.9%	Standard projects – GA CR
0.6%	International grant projects evaluated on the LEAD Agency principle – GA CR
0.6%	EPSILON program for the support of applied research and experimental development – TA CR
0.3%	Security research of the Czech Republic – MI
0.1%	Researcher Mobility support within international cooperation in R&D&I – MEYS

Operational and Capital Expenditures



The total expenditures of IT4Innovations amounted to CZK 311,218,000. Within this amount, non-investment (operational) expenses and investment (capital) expenses amounted to 70.1% and 29.9%, respectively. The largest part of operational expenses included personnel expenses, services (power consumption, maintenance service for the operated supercomputing systems and the related infrastructure, technical and system support, etc.) overhead expenses, and membership fees (in international organizations and consortia such as PRACE, ETP4HPC, EUDAT, BDVA, and LUMI).

34.4%	Personnel costs – research teams
17.8%	Services
17.2%	Personnel costs – management, administration, and supercomputing services
12.6%	Overhead costs
12.2%	Fees
3.9%	International and domestic business trips (including those of invited speakers)
0.7%	Small tangible fixed assets
0.6%	Consumables
0.5%	Scholarships

93.3%	Tangible fixed assets – machines and equipment
6.0%	Intangible fixed assets
0.7%	Other tangible fixed assets

Summary of All Grants

- SUPERCOMPUTING SERVICES
- RESEARCH AND DEVELOPMENT
- EDUCATIONAL AND TRAINING ACTIVITIES

National Grants

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

Large Infrastructures Project for Research, Experimental Development, and Innovation

- IT4Innovations National Supercomputing Center

National Programme of Sustainability II

- IT4Innovations Excellence in Science

Grants for specific university research for 2019 – SGC

- Incoherent Effects in Multilayer Structures with Lateral Periodicity
- Advanced Modelling of Materials and Multiscale Modulated Nanostructures
- Quantification and Qualification Tool's Application to Dynamical Systems
- Extension of HPC Platforms for Executing Scientific Pipelines
- Internationalization of Doctoral Education in Molecular Physics II
- Infrastructure Research and Development of HPC Libraries and Tools
- Using HPC to Solve Engineering Problems

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

- Modeling of Interactions of Cold Rare-gas Plasmas with Ambient Air
- Metal-graphene Interfaces – Foundations of Novel Spintronic Materials
- Understanding of the Magnetostriction in Fe-Ti Alloys by First-principles Calculations
- Physics of Phononic Interactions in Solids for Terahertz Light Generation

Projects of Operational Programme Research, Development and Education

- IT4Innovations National Supercomputing Center – Path to Exascale
- Doctoral School for Education in Mathematical Methods and Tools in HPC
- Technology for the Future
- Technology for the Future 2.0
- Artificial Intelligence and Reasoning
- Science without Borders

Projects supported by the Grant Agency of the Czech Republic

- Novel Fuel Materials for the IV Generation Nuclear Reactors
- Space-time Boundary Element Methods for the Heat Equation

Projects supported by the Technology Agency of the Czech Republic

- Parallelized Reaction-transport Model for Contamination Spread in Groundwater
- Centre of Competence for Molecular Diagnostics and Personalized Medicine
- Personalized Medicine – Diagnostics and a Therapy
- Optimization of the Electrical Distribution System Operating Parameters Using Artificial Intelligence
- Contactless Detector for Partial Discharge Activity in Medium Overhead Voltage Powerlines
- National Centre for Energy (NCE)
- Energy Systems for Grids

Projects supported by the Ministry of Industry and Trade

- Intake and Discharge Objects of Pump and Turbine Stations
- Digital Twin of Product within Siemens Plants

Projects supported by the Ministry of Interior

- Employment of Artificial Intelligence into an Emergency Call Reception

International Grants

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

- PRACE-5IP – Partnership for Advanced Computing in Europe, 5th Implementation Phase
- EXPERTISE – Experiments and High-Performance Computing for Turbine Mechanical Integrity and Structural Dynamics in Europe
- TETRAMAX – Technology Transfer via Multinational Application Experiments
- CloudiFacturing – Cloudification of Production Engineering for Predictive Digital Manufacturing
- ExaQUte – Exascale Quantifications of Uncertainties for Technology and Science Simulation
- POP2 – Performance Optimisation and Productivity 2
- NEW LEXIS – Large-scale EXecution for Industry & Society
- NEW OPENQKD – Open European Quantum Key Distribution Testbed
- NEW PRACE-6IP – Partnership for Advanced Computing in Europe, 6th Implementation Phase

Project of the Interreg Danube Transnational Programme (EU funds)

- InnoHPC – High-Performance Computing for Effective Innovation in the Danube Region

International Visegrad Fund

- Superheroes 4 Science

SUPERCOMPUTING SERVICES

IT4Innovations operates four supercomputers: Anselm (94 TFlop/s, installed in summer 2013), Salomon (2 PFlop/s, installed in summer 2015), Barbora (849 TFlop/s, installed in autumn 2019), and the NVIDIA DGX-2 system specialized for Artificial Intelligence calculations (130 TFlop/s and 2 PFlop/s for AI, installed in spring 2019). The two newest supercomputers operated by IT4Innovations were procured within the **IT4Innovations national supercomputing center – path to exascale project** supported by the Operational Programme Research, Development, and Education of the Ministry of Education, Youth and Sports of the Czech Republic.

In 2019, IT4Innovations started to actively participate in the EuroHPC JU project, in the frame of which a **new petascale supercomputer** entitled EURO_IT4I with a theoretical peak performance of about 13.6 PFlop/s will be installed in 2020. With its parameters, this supercomputing system will rank among the most powerful supercomputers in Europe. The system will be designed to meet user requirements for solving complex scientific and engineering problems such as classical numerical simulations, big data analysis, and use of Artificial Intelligence.

Simultaneously, IT4Innovations achieved success in the competition to build a EuroHPC pre-exascale supercomputing system as a member of the **LUMI (Large Unified Modern Infrastructure) consortium** formed by Finland as the Coordinator, Belgium, Denmark, Estonia, the Netherlands, Norway, Poland, Sweden, and Switzerland. By the end of the year 2020, the system will have been installed in Kajaani, Finland, and will become one of the most powerful systems in Europe as well as worldwide.

Technical Specifications of the Supercomputers

	Anselm	Salomon	NVIDIA DGX-2	Barbora
Put into operation	Spring 2013	Summer 2015	Spring 2019	Autumn 2019
Theoretical peak performance	94 TFlop/s	2,011 TFlop/s	130 TFlop/s 2 PFlop/s pro AI	849 TFlop/s
Operating system	RedHat Linux 64bit 6.x	CentOS 64bit 7.x	CentOS 64bit 7.x	CentOS 64bit 7.x
Compute nodes	209	1,008	1	201
CPU	2 x Intel SandyBridge, 8 cores, 2.3 / 2.4 GHz, 3,344 cores in total	2 x Intel Haswell, 12 cores, 2.5 GHz, 24,192 cores in total	2 x Intel Xeon Platinum, 24 cores, 48 cores in total	2 x Intel Cascade Lake, 18 cores, 2.6 GHz
RAM per compute node	64 GB / 96 GB / 512 GB	128 GB / 3.25 TB (UV node)	1.5 TB DDR4, 512 GB HBM2 (16 x 32 GB)	192 GB / 6 TB fat node
GPU accelerators	23 x NVIDIA Tesla K20 (Kepler)	N/A	16 x NVIDIA Tesla V100 / 32 GB HBM2	32 x NVIDIA Tesla V100
MIC accelerators	4 x Intel Xeon Phi 5110P	864 x Intel Xeon Phi 7120P	N/A	N/A
Storage	320 TiB / home (2 GB/s), 146 TiB / scratch (6 GB/s)	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)
Interconnection	Infiniband QDR 40 Gb/s	Infiniband FDR 56 Gb/s	8 x Infiniband nebo 8 x 100 GbE	Infiniband HDR 200 Gb/s

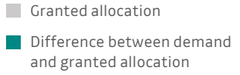
Computational Resources Allocation

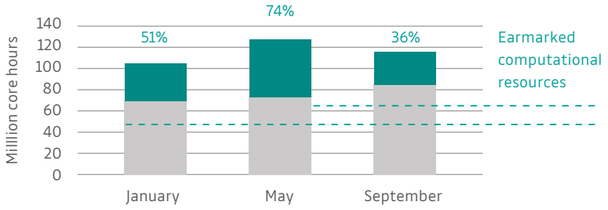
The computational resources of IT4Innovations are dedicated to solving problems in research and development conducted primarily by academic and research institutions. Unused capacity can be freed up for the development of collaboration between academia and industry as well as for purely commercial use.

In 2019, IT4Innovations provided its computational resources to 190 projects within the Open Access Grant Competition and to 39 projects through the Directors' Discretion scheme. A total of 253,412,910 core hours were allocated with 94% and 6% being allocated within three Open Access Grant Competitions and through the Directors' Discretion scheme, respectively. The total allocation of computational resources through the Directors' Discretion scheme includes both the PRACE DECI Calls and commercial sector allocations.

A core hour refers to the number of processor units (cores) used to run a simulation multiplied by the duration of the job in hours.

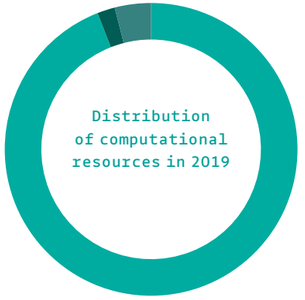
Open Access Grant Competitions in 2019



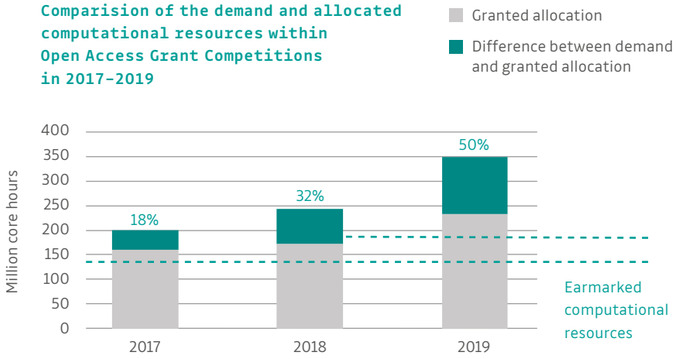


Open Access Grant Competitions

Institutions can apply for computational resources within Open Access Grant Competitions. These are announced three times a year. In 2019, more than 233 million core hours were allocated and distributed across 190 research projects within three Open Access Grant Competitions, enhancing Czech science. Given the increasing demand and procurement of new supercomputing systems during the year, the computational resources earmarked for each Open Access Grant Competition were gradually increased from 48 up to 66 million core hours. Throughout the year, the aggregated reserved capacity was increased from 144 to 180 million core hours. In 2017 and 2018, the excess demand for core hours over the available capacity amounted to more than 39% and almost 70%, respectively. In 2019, in contrast, it was 96%. In the last three years, almost 856 million core hours were distributed across 496 projects within the Open Access Grant Competitions. Most computational resources, i.e. 50.5%, were awarded to projects in the field of material science and biosciences. Committee found most of the submitted applications scientifically and technically thoroughly elaborated. However, for the reason of insufficient capacity, the computational resources awarded to each project had to be reduced. The difference between the core hour demand and the computational resources reserved for the Open Access Grant Competitions is compensated by the reserves available through the Directors' Discretion scheme as well as the IT4Innovations system administration. In 2019, the difference between the demand and the allocated amount was approximately 54%.



Comparision of the demand and allocated computational resources within Open Access Grant Competitions in 2017–2019

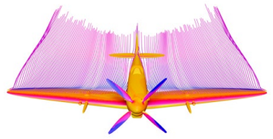


Year	Earmarked resources (corehours)	Difference between demand and earmarked computational recource	Difference between demand and granted allocation
2017	144 million	39%	25%
2018	144 million	70%	42%
2019	180 million	96%	54%

Results of the Open Access Grant Competitions in 2019

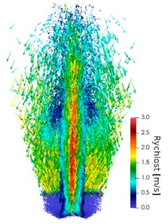
Within the Open Access Grant Competitions in 2019, a total of 55 projects of applicants from VSB – Technical University of Ostrava were awarded computational resources amounting to approximately 52 million core hours. A total of 12 projects were led by researchers from the Faculty of Civil Engineering, the Faculty of Electrical Engineering and Computer Science, the Nanotechnology Centre, the Faculty of Mechanical Engineering, and the Faculty of Materials Science and Technology. The remaining 43 projects were led by researchers from IT4Innovations, a university institute of VSB-TUO. Concerning the external research institutions using the IT4Innovations infrastructure, most of the computational resources were allocated for the projects of researchers affiliated with the Czech Academy of Sciences (CAS). Its 10 institutes were awarded 57.6 million core hours for a total of 44 projects. Most of the computational resources were allocated to the projects of the Institute of Organic Chemistry and Biochemistry and the J. Heyrovsky Institute of Physical Chemistry. Almost ten million core hours or more were also awarded to other institutes, namely CEITEC, Charles University, the Czech University of Life Sciences Prague (CULS Prague), and Masaryk University.

Results of the 15th Open Access Grant Competition in Q1/2019 Newsletter



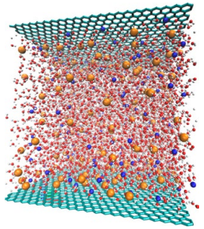
Research and Development of Libraries and Tools in the INFRA Lab and the project of Dr Petr Strakoš and Dr Lubomír Říha from IT4Innovations

Machine Learning in Biometrics and Biomedicine and the project of Jan Tinka from Brno University of Technology

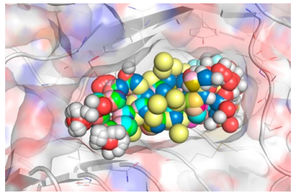


Investigation of Fluidization Regimes in Wurster Fluid Bed Coater and the project of Jiří Kolář from University of Chemistry and Technology, Prague

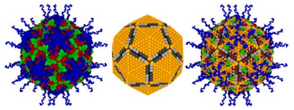
Results of the 16th Open Access Grant Competition in Q2/2019 Newsletter



Molecular and Mesoscopic Simulations of Aqueous Solutions in Inhomogeneous Enviroments and the project of Dr Barbora Planková from the Czech Academy of Sciences

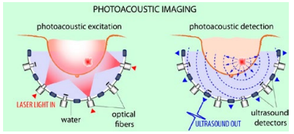


Virtual Screening of Human and Plant Hormones and the project of Dr Václav Bazgier from Palacký University in Olomouc

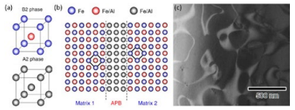


Mechanism of Genome Release of Non-Enveloped Viruses and the project of Lukáš Sukeník from CEITEC, Masaryk University

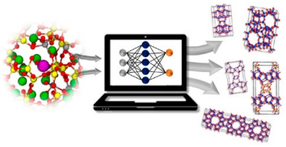
Results of the 17th Open Access Grant Competition in Q4/2019 Newsletter



Photoacoustic Tomography of the Breast and the project of Doc. Jiří Jaroš from Brno University of Technology



From Antiphase Boundaries to New Rare-Earth-Free Magnets and the project of Prof. Mojmír Šob from CEITEC, Masaryk University

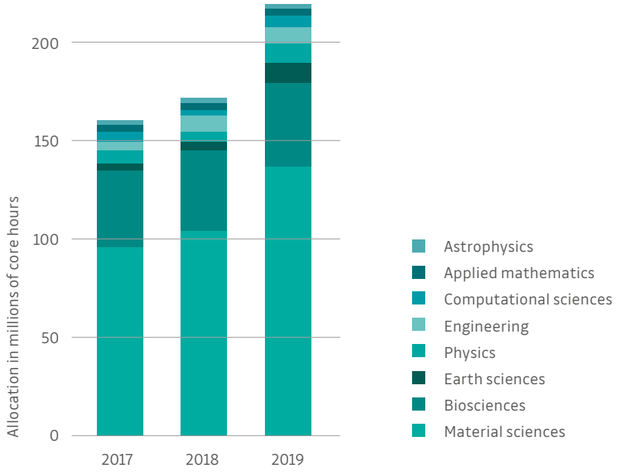


Neural Network Potentials for in silico Design of Zeolites and the project of Dr Lukáš Grajciar from Charles University

25.3%	Czech Academy of Sciences institutes
21.4%	VSB – Technical University of Ostrava
14.8%	CEITEC
13.5%	Charles University
7.9%	The Czech Technical University in Prague
5.7%	Masaryk University
3.4%	Brno University of Technology
3.2%	University of Chemistry and Technology, Prague
2.8%	The University of Ostrava
2%	Others

62.4%	Material sciences
19.4%	Biosciences
4.7%	Earth sciences
4.5%	Physics
3.8%	Engineering
2.6%	Computational sciences
2.0%	Applied mathematics
0.5%	Astrophysics

Allocation of computational resources in 2017, 2018, and 2019 by scientific discipline



Directors' Discretion

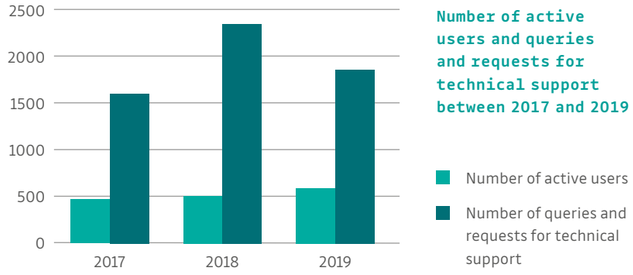
Furthermore, 6% of the IT4Innovations computational resources can also be granted to projects upon request within the Directors' Discretion scheme. Applications can be submitted at any time. The computational resources are allocated irregularly based on evaluation by the IT4Innovations management. Representatives from the non-commercial sector can apply in case Open Access Grant Competitions cannot be used. Within the Directors' Discretion scheme in 2018, a total of 17 projects were allocated 4 million core hours. Within the Directors' Discretion scheme in 2019, a total of 39 projects were allocated more than 15 million core hours. These projects also included those of applicants from the commercial sector, who also have the opportunity to rent the computational resources. In 2019, 9 companies concluded rental agreements amounting to approximately 4.9 million corehours.

Users of Computational Resources

In 2019, the number of active users was 591 in total. In comparison with the year 2018, this increased by 16%.

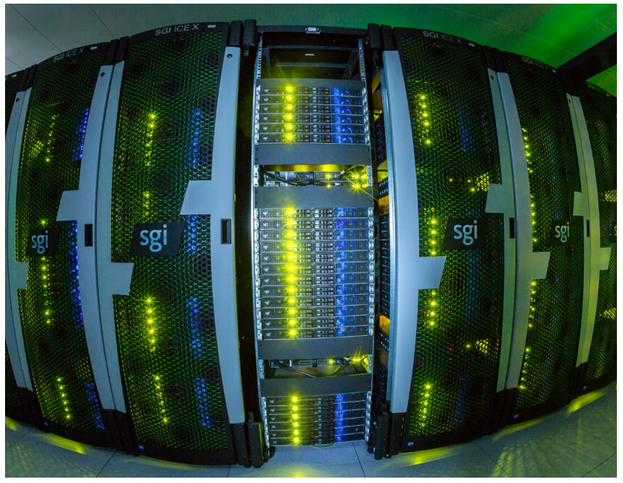
In 2019, the IT4Innovations Technical Support received 1,839 queries and requests. The internal response time (24 h for the first response) was observed in 99.95% of queries. The internal closure time, which should not be longer than 30 days, was observed in 99.30% of queries.

Number of active users and queries and requests for technical support between 2017 and 2019



Supercomputing Services Projects

Several national and international grants help IT4Innovations secure operation and development of its supercomputing infrastructure. In terms of operation of the current systems, the most important one is the grant from the Ministry of Education, Youth and Sports of the Czech Republic (MEYS) – IT4Innovations National Supercomputing Center, which is funded by sources dedicated to supporting Large Infrastructures for Research, Experimental Development, and Innovation. Modernization of the IT4Innovations computational capacity is funded by the Operational Programme Research, Development, and Education of MEYS, in particular, by the IT4Innovations national supercomputing center – path to exascale project. The important international projects we are involved in thanks to our participation in the Partnership for Advanced Computing in Europe (PRACE) include the eponymous infrastructure projects funded by the European Commission Horizon 2020 programme. In 2019, the 6th implementation phase of the project titled PRACE-6IP was launched.



National Grants

Projects supported by Ministry of Education, Youth and Sports

IT4Innovations National Supercomputing Center (2016–2019)

PROJECT ID
LM2015070 ((Large Infrastructures for Research and Experimental Development and Innovations project)

PRINCIPAL INVESTIGATOR
Doc. Vít Vondrák

The objective of the project is to operate the most powerful, state-of-the-art supercomputing systems in the Czech Republic and provide open access to these resources based on research excellence.

Necessary for providing the aforementioned computing capacities is the operation of the related infrastructure (power supply, cooling, safety, fire protection, etc.), as well as user support and the management of computing and infrastructure systems. In addition, research activities that streamline its operation and extend its use to the user are also part of the project. The educational and training activities that are open to the broader scientific community of the Czech Republic also contribute to effective use of the infrastructure.

International Grants

IT4Innovations National Supercomputing Center – path to exascale (2017–2021)

PROJECT ID
EF16_013/0001791 (call no. 02_16_013 Research Infrastructure)

PRINCIPAL INVESTIGATOR
Dr Branislav Jansík

The objective of this project is to upgrade and modernize the research infrastructure of IT4Innovations so as to at the very least maintain the existing technological level of HPC in the Czech Republic in comparison with developed, particularly European, countries. The activities of this project are aimed at modernizing the equipment and supplementing the current Anselm supercomputer with a similar modern supercomputer (Small cluster) in terms of extent and function in 2018. In 2020, a new supercomputer, exceeding the capacity of Salomon, the most powerful system of IT4Innovations so far, is to be procured. 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.

PRACE-5IP – Partnership for Advanced Computing in Europe, 5th implementation phase (2017–2019)

PROJECT ID
730913 (call no. H2020-EINFRA-2016-1)

PRINCIPAL INVESTIGATOR
Doc. Vít Vondrák

NEW

PRACE-6IP – Partnership for Advanced Computing in Europe, 6th implementation phase (2019–2021)

PROJECT ID 823767
(call no. H2020-INFRAEDI-2018-2020)

PRINCIPAL INVESTIGATOR
Doc. Vít Vondrák

The objectives of the PRACE (Partnership For Advanced Computing in Europe) projects are to build on the successful implementation of the previous PRACE projects, whose task was to implement the European HPC infrastructure and to continue to develop supercomputing cooperation to strengthen the competitiveness of European science, research and industry.

InnoHPC – High Performance Computing for Effective Innovation in the Danube Region (2017–2019)

PROJECT ID
DTP1-1-260-1.1 (INTERREG/Danube region programme, 1st call)

PRINCIPAL INVESTIGATOR
Dr Tomáš Karásek

The objective of the InnoHPC project is to design a transnational HPC platform for developing cooperation of research institutions with small and medium-sized enterprises. The participating enterprises will be allowed access to supercomputing infrastructures. The participating research institutions, on the other hand, will gain an opportunity to collaborate in solving real world problems and use their entrepreneurial potential.

RESEARCH AND DEVELOPMENT

IT4Innovations conducts excellent research in the field of high-performance computing, big data processing, and artificial intelligence.

The main research areas of IT4Innovations include big data processing and analysis, machine learning, development of parallel scalable algorithms, solution of computationally demanding engineering problems, advanced visualization, 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 organizations (PRACE, ETP4HPC, BDVA, I4MS, HiPEAC, and EUDAT CDI). It is also involved in implementing more than a dozen international projects funded primarily by the Horizon 2020 programme. IT4Innovations is the Coordinator of the H2020 LEXIS project as well as a member of the H2020 POP2 Centre of Excellence and the FETHPC ExaQUte project. Moreover, IT4Innovations is involved in development of the European Space Agency (ESA) funded Urban Thematic Exploitation Platform, and in the past it participated in a number of projects supported by the FP7 and H2020 programs such as PRACE, EXA2CT, HARPA, ExCAPE, ANTAREX, READEX, SESAME NET, and many others.

71.3%	NANO
14%	PAR
9.3%	ADAS
2.8%	INFRA
2.6%	BIG DATA

IT4Innovations Research is conducted in five laboratories:

- PARALLEL ALGORITHMS RESEARCH LAB
- ADVANCED DATA ANALYSIS AND SIMULATIONS LAB
- MODELLING FOR NANOTECHNOLOGIES LAB
- BIG DATA ANALYSIS LAB
- INFRASTRUCTURE RESEARCH LAB

In 2019, 42 projects of the IT4Innovations research labs were allocated more than 55 million core hours, which is 23% of the aggregated allocated amount, within the Open Access Grant Competitions. Most projects were submitted by the researchers from the Parallel Algorithms Research Lab, and most computational resources were awarded to the Modelling for Nanotechnologies Lab.

Research and Development Flagships

In 2019, 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. The IT4Innovations flagships include 3 projects:

ESPRESO - Highly Parallel Finite Element Package for Engineering Simulations

RESEARCHER Dr Tomáš Brzobohatý

The latest technological advances in computing have brought a significant change in the concept of new product design, production control, or autonomous systems. In the last few years, we have been witnessing the considerable transition to virtual prototyping and gradual pressure on integrating large part of the industrial sector in the fourth industrial revolution. The main objective of the flagship is to create a robust open-source package ESPRESO applicable for a wide range of complex engineering simulations in areas such as mechanical engineering, civil engineering, biomechanics, and energy industry. The open-source approach allows automatized simulation chains, based on HPC-as-a-service, such as automatized systems for shape or topological optimization which will be created on the top of the ESPRESO framework. For all the framework components, development of highly scalable methods allowing full utilization of the computational capacity of state-of-the-art supercomputers will be strictly enforced. This work ena- bles to enlarge the IT4Innovations portfolio of services offered to industry and extend the IT4Innovations HPC demonstrators based on real applications.

Material design - Towards Reality via Exascale Computing

RESEARCHER Dr Dominik Legut

Since the advances in HPC the simulation of material behavior has played a key role in our lives. This fact was even more pronounced once there was a way to perform quantum mechanical calculations to obtain electronic structure of materials and its behavior to link to many physical and chemical properties. First-principles (ab initio) calculations at present are the parameter free approach for i) verification of the experiments ii) to simulate conditions or calculate material properties that are not directly accessible or measurable iii) to design novel materials. Within the flagship we address fundamental and state-of-the-art topics like to design nuclear fuels materials from radioactive compounds for IVth generation nuclear reactors, ultrafast magnetization 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

RESEARCHER
Dr Jan Martinovič
and Dr Stanislav Böhm

The main goal of the most supercomputing centres is to lower the entry barriers to the world of HPC 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 which 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 the hardware. Simultaneously, large portion of HPC workloads are 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 programing 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.

Parallel Algorithms Research Lab

The lab is focused on high-quality basic and applied research in the field of development of scalable algorithms and HPC libraries, numerical modelling, engineering simulations, and high-performance molecular simulations.

HEAD OF LAB:
Dr Tomáš Karásek

NUMBER OF EMPLOYEES: 23

Significant events

- The IT4Innovations Digital Innovation Hub was awarded the **best DIH of November by DIHnet EU**.
- Completion and successful defense of the **InnoHPC** project, the objective of which was to develop a multinational HPC platform for developing cooperation between research institutions and enterprises focused on small and medium-sized enterprises.
- **Contract research** concluded with the ING Corporation, spol. s r.o., Glass Service a.s., and Siemens s.r.o. companies.

Selected publications

- Brzobohatý T., Jarošová M., Kučera R., Šátek V. Path-Following Interior Point Method: Theory and Applications for the Stokes Flow with a Stick-Slip Boundary Condition. Advances in Engineering Software, roč. 2019, č. 129, s. 35-43. ISSN 0965-9978. DOI: 10.1016/j.advengsoft.2018.06.010, IF: 4.194
- Van de Steen, C., Benhenni, M., Kalus, R., Ćosić, R., Gadea, F.X., Yousfi, M., Mobility and Dissociation of Electronically Excited ${\mathrm{Kr}}_{2}^{+}$ Ions in Cold Krypton Plasma. Plasma Source Sci. Technol. DOI: 10.1088/1361-6595/ab3a17, IF: 4.128
- Van de Steen, C., Benhenni, M., Kalus, R., Ćosić, R., Iléssová, S., Gadea, F.X., Yousfi, M., Calculations of Cross-Sections, Dissociation Rate Constants and Transport Coefficients of Xe2+ Colliding with Xe. Phys. Chem. Chem. Phys. DOI: 10.1039/c9cp00338j, IF: 3.567
- Zapoměl, J., Ferfecki, P., Kozánek J.: The Mathematical Model for Analysis of Attenuation of Nonlinear Vibration of Rigid Rotors Influenced byEelectromagnetic Effects, Journal of Sound and Vibration, Volume 443, 17 March 2019, 167-177. DOI: 10.1016/j.jsv.2018.11.008, IF: 3.123
- Kravčenko, M., Merta, M., Zapletal, J.: Distributed Fast Boundary Element Methods for Helmholtz Problems. Applied Mathematics and Computation. DOI: 10.1016/j.amc.2019.06.017, IF: 3.092

Advanced Data Analysis and Simulation Lab

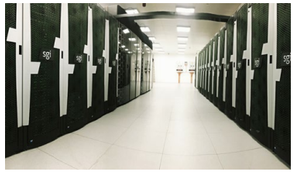
The lab specializes in advanced data analysis, research and development in the field of HPC co-design, data and cloud technologies to enhance industry and society, programing models for HPDA, Artificial Intelligence, modelling, simulation, and application of dynamical systems.

HEAD OF LAB:
Dr Jan Martinovič

NUMBER OF EMPLOYEES: 36

Significant events

- Commencement of the **LEXIS** project of which IT4Innovations is the Coordinator. The objective of the project is 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 will be demonstrated via three pilot tests suitable for industrial fields involving such things as aerospace, weather and climate, and earthquakes and tsunami.



- Participation in the activities of the **Big Data Value Association** and the **Private Public Parthership** via the LEXIS project.
- Active participation with partners within the **EUDAT Collaborative Data Infrastructure**.
- Participation in negotiations and activities of the Research and Innovation Advisory Group within **EuroHPC JU**.
- The **BLENDED** project accepted for the European Space Agency (ESA). The main objective of the project is to investigate possibilities as well as to report on synergic use of Blockchain and Deep Learning technologies for space data.
- Successful completion of the H2020 **ANTAREX** project focused on a self-adaptive approach for applications run on supercomputers and publishing of the results achieved.
- Tomáš Martinovič won the **Best Poster Award at the ISC 2019 conference** for his contribution entitled HPC Oriented Algorithm for Computation of Recurrence Quantitative Analysis.
- **Two articles** by Jakub Beránek dealing with network-accelerated non-contiguous memory transfers and interface design for FPGA communication were published at the SC19 conference.

Selected publications

- Ueda, H.R., Ertürk, A., Chung, K. et al. Tissue Clearing and its Applications in Neuroscience. Nat Rev Neurosci 21, 61–79 (2020) DOI: 10.1038/s41583-019-0250-1, IF: 33.162
- Kožusznik, J., Bainar, P., Klímová, K., Krumnikl, M., Moravec, P., Svatoň, V., Tomančák, P. SPIM Workflow Manager for HPC, Bioinformatics, Volume 35, Issue 19, 1 October 2019, Pages 3875–3876, DOI: 10.1093/bioinformatics/btz140, IF: 4.531
- Haase, R., Royer, L.A., Steinbach, P. et al. CLIJ: GPU-Accelerated Image Processing for Everyone. Nat Methods 17, 5–6 (2020) DOI: 10.1038/s41592-019-0650-1, IF: 4.170
- Brkić, D.; Praks, P. Short Overview of Early Developments of the Hardy Cross Type Methods for Computation of Flow Distribution in Pipe Networks. Appl. Sci. 2019, 9, 2019. DOI: 10.3390/app9102019, IF: 2.217
- Brkić, D.; Praks, P. Accurate and Efficient Explicit Approximations of the Colebrook Flow Friction Equation Based on the Wright ω-Function. Mathematics 2019, 7, 34. DOI: 10.3390/math7010034, IF: 1.105

Modelling for Nanotechnologies Lab

The lab is focused on optical diagnostics, novel material design, development of special surfaces for nanooptics, and modelling and design of nanocomposites.

HEAD OF LAB:
Prof. Jaromír Pištora

NUMBER OF EMPLOYEES: 16

Significant events

- Organization of the **Czech-French workshop** focused on nanotechnologies, which was held at IT4Innovations.
- Barbora Kacerovská was announced the winner of the **Lady Business** competition in the Exceptional Student of the Moravian-Silesian Region category.
- **Contract research** conducted for the Continental company in the field of design and application of new materials.
- Award of a new H2020 project entitled **s-NEBULA**, which is aimed at development of new spin-based building blocks using spin electronic properties for generation and detection of terahertz radiation and advanced terahertz applications.

Selected publications

- Fu, Z. H., Wang, N., Legut, D., Si, Zhang, Q.F., Du, S.Y., Germann, T.C., Francisco, J.S., Zhang, R. F.: Rational Design of Flexible Two-Dimensional MXenes with Multiple Functionalities.CHEMICAL REVIEWS 119, no. 23, (2019). DOI: 10.1021/acs.chemrev.9b00348, IF: 54.301.
- Zhang, R.F., Zhang, S.H., Guo, Y.Q. , Fu, Z.H., Legut, D., Germann, T.C., Veprek, S.: First-Principles Design of Strong Solids: Approaches and applications. PHYSICS REPORTS-REVIEW SECTION OF PHYSICS LETTERS 826, (2019). DOI: 10.1016/j.physrep.2019.09.004, IF: 28.295
- Xiao, J.W., Zhou, G.M., Chen, H.T., Feng, X., Legut, D., Fan, Y.C., Wang, T.S., Cui, Y., Zhang, Q.F.: Elaboration of Aggregated Polysulfide Phases: From Molecules to Large Clusters and Solid Phases. NANO LETTERS 19, no. 10, (2019). DOI: 10.1021/acs.nanolett.9b03297, IF: 12.279
- Chen, H.T., Handoko, A.D., Xiao, J.W., Feng, X., Fan, Y.C., Wang, T.S., Legut, D., Seh, Z.W., Zhang, Q.F.: Catalytic Effect on CO2 Electroreduction by Hydroxyl-Terminated Two-Dimensional MXenes. ACS APPLIED MATERIALS & INTERFACES 11, (2019). DOI: 10.1021/acsami.9b09941, IF: 8.456
- Guo, Y.Q., Zhang, S.H., Zhan, B., Beyerlein, I.J., Legut, D., Shang, S.L., Liu, Z.K., Zhang, R.F.: Synergetic Effects of Solute and Strain in Biocompatible Zn-Based and Mg-Based Alloys. ACTA MATERIALIA 181, (2019). DOI: 10.1016/j.actamat.2019.09.059, IF: 7.293
- Nguyen-Huu, N., Pištora, J., Cada, M.: Dual Broadband Infrared Absorptance Enhanced by Magnetic Polaritons Using Graphene-Covered Compound Metal Gratings. Optics Express 27, (2019), DOI: 10.1364/OE.27.030182, IF: 3.561
- Vlček, J., Pištora, J., Lesňák, M.: Design of Plasmonic-Waveguiding Structures for Sensor Applications. Nanomaterials 9, (2019), DOI: 10.3390/nano9091227, IF: 4.034

Big Data Analysis Lab

The lab focuses on network security, Internet of Things, big data analysis, speech processing as well as Artificial Intelligence applications in complex systems.

HEAD OF LAB:
Prof. Miroslav Vozňák

NUMBER OF EMPLOYEES: 8

Significant events

- Launching of the **OPENQKD** project. The project aims at establishing a testbed for a highly-secure network using principles of quantum mechanics for key distribution. The three year-long project is the largest implementation of QKD (Quantum Key Distribution) in Europe so far.
- The research team led by Ivan Zelinka received an honorary award from the expert panel within the **Visionaries 2019** project competition for their Chiméra mobile application for encrypted communication.
- **Contract research** for the National Cyber and Information Security Agency.

Selected publications

- Skanderova, L., Fabian, T., Zelinka, I. Self-Adapting Self-Organizing Migrating Algorithm (2019) Swarm and Evolutionary Computation, 51, art.no.100593. DOI: 10.1016/j.swevo.2019.100593, IF: 6.33
- Chamorro, H.R., Sanchez, A.C., Pantoja, A., Zelinka, I., Gonzalez-Longatt, F., Sood, V.K. A Network Control System For Hydro Plants to Counteract the Non-Synchronous Generation Integration (2019) International Journal of Electrical Power and Energy Systems, 105, pp. 404-419. DOI: 10.1016/j.ijepes.2018.08.020, IF: 4.418
- Chamorro, H.R., Riaño, I., Gerndt, R., Zelinka, I., Gonzalez-Longatt, F., Sood, V.K. Synthetic Inertia Control Based on Fuzzy Adaptive Differential Evolution (2019) International Journal of Electrical Power and Energy Systems, 105, pp. 803-813. DOI: 10.1016/j.ijepes.2018.09.009, IF: 4.418
- Keles, H.Y., Rozhon, J., Gokhan Ilk, H., Voznak, M. DeepVoCoder: A CNN Model for Compression and Coding of Narrow Band Speech (2019) IEEE Access, 7, art. no. 8730308, pp. 75081-75089. DOI: 10.1109/ACCESS.2019.2920663, IF: 4.098
- Huynh, V.-V., Nguyen, H.-S., Hoc, L.T.T., Nguyen, T.-S., Voznak, M. Optimization Issues for Data Rate in Energy Harvesting Relay-Enabled Cognitive Sensor Networks (2019) Computer Networks, 157, pp. 29-40. DOI: 10.1016/j.comnet.2019.04.012, IF: 3.03
- Snasel, V., Kromer, P., Safarik, J., Platos, J. JPEG Steganography with Particle Swarm Optimization Accelerated by AVX (2020) Concurrency Computation, 32 (8), art. no. e5448. DOI: 10.1002/cpe.5448, IF: 1.167

Infrastructure Research Lab

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

HEAD OF LAB:
Dr Lubomír Říha

NUMBER OF EMPLOYEES: 12

Significant events

- Award of a **TA CR-funded project aimed** at developing a functional sample of a railway vehicle capable of detecting obstacles in the driving profile by means of a set of HW sensors, a sophisticated data processing architecture, and artificial intelligence tools for final identification of obstacles and their subsequent interpretation to the locomotive driver. As a key support for development and optimization of the detection system, the project includes development of a software simulator for virtualization of railway conditions as well as implementation of test rides in a laboratory environment.
- Organization of a special section focused on Tools for Energy Efficient Computing at the international **PPAM 2019** conference.
- Participation in the international **PowerStack** initiative addressing the topic of HPC systems energy efficiency.
- Cooperation in preparing the PRACE Energy Efficiency in HPC worshop held at the CINECA supercomputing centre in Italy.
- Preparation of the PTC Parallel Visualization of Scientific Data Using Blender course, cooperation in preparing the PTC Developing Efficient HPC Applications for the Latest CPU Architectures with C++ and Fortran course.
- Publikace softwaru: Meca, O., Říha, L., Brzobohatý, T.: **Software tool MESIO**.
- Publikace softwaru: Jaroš, M., Strakoš, P., Říha, L.: **Software tool CyclesPhi**.
- Publikace softwaru: Peterek, I., Beseda, M., Vysocký, O.: **Software tool RADAR visualize**.

Important conference contributions

- Meca O., Říha L. and Brzobohatý T. An Approach for Parallel Loading and Pre-Processing of Unstructured Meshes Stored in Spatially Scattered Fashion, 2019 IEEE International Parallel and Distributed Processing Symposium (IPDPS), Rio de Janeiro, Brazil, 2019, pp. 749-760. DOI: 10.1109/IPDPS.2019.00084
- O. Vysocký, L. Říha, A. Bartolini: Overview of Application Instrumentation for Performance Analysis and Tuning (2019) Proceedings of The International Conference on Parallel Processing and Applied Mathematics, PPAM 2019
- Kovács L., Strakoš P., Jaroš M., Kovács R., Kovács-Sós A., Karásek T., Hajdu A. Hybrid Small Size High Performance Computing Resource for Medical Image Analysis, in Iványi P., Topping B.H.V. Proceedings of the Sixth International Conference on Parallel, Distributed, GPU and Cloud Computing for Engineering, Civil-Comp Press, Stirlingshire, UK, Paper 28, 2019. DOI: 10.4203/ccp.112.28
- Jaroš M., Vysocký O., Strakoš P., Špeťko M. Energy Consumption Evaluation of Blender's Image Renderer in HPC Environment, in Iványi P., Topping B.H.V. Proceedings of the Sixth International Conference on Parallel, Distributed, GPU and Cloud Computing for Engineering, Civil-Comp Press, Stirlingshire, UK, Paper 32, 2019. DOI: 10.4203/ccp.112.32

National Grants

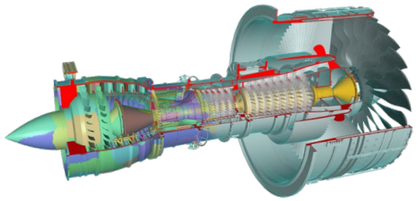
Projects supported by the Ministry of Education, Youth and Sports

IT4Innovations Excellence in Science (2016–2020)

PROJECT ID LQ1602

PRINCIPAL INVESTIGATOR
Prof. Tomáš Kozubek

In the years 2011 to 2015, the IT4Innovations Centre of Excellence project was jointly implemented by the following partners: VSB – Technical University of Ostrava, the University of Ostrava, the Silesian University in Opava, Brno Technical University, and the Institute of Geonics of the Czech Academy of Sciences. The cooperation of these institutions is currently continuing within the National Programme of Sustainability II (IT4Innovations excellence in science) by conducting excellent research in the fields of high performance computing and cyberphysical systems.



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

Modeling of Interactions of Cold Rare-gas Plasmas with Ambient Air (2018–2019)

PROJECT ID 8J18FR031

PRINCIPAL INVESTIGATOR
Doc. René Kalus

The project aims at performing extensive ab initio calculations to deeply understand the interactions in [He/X2]+(X = N, O) collision systems including excited electronic states and transitions between them. Another objective is to create a suite of codes for non-adiabatic dynamics simulations linking hybrid dynamical approaches with on-the-fly ab initio calculations. Using the codes created within the project, pilot dynamical calculations on a selected collision systems, He+/X2 (X = N, O) will be performed, with the main aim to get collision cross-sections to be further used in macroscopic modelings. The collision cross-sections will be used in calculations of transport properties (mobilities) of He+ions in X2 (X = N, O). The reliability of the theoretical approaches will be compared against experimental data.

Metal-graphene Interfaces – Foundations of Novel Spintronic Materials (2018–2019)

PROJECT ID 8J18DE004

PRINCIPAL INVESTIGATOR
Dr Dominik Legut

The main objective of this study is the investigation of magnetization effects in graphene induced by magnetic layers like Co, Ni, Fe-alloys, e.g. FeCo. The applied spectroscopy is reflection polarization spectroscopy and total electron yield (absorption) spectroscopy with soft x-ray synchrotron radiation across the carbon 1s resonance energy. This advance topic follows the basic optical characterization (optical constants) by means of the theoretically calculated and experimentally measured magneto-optical effects of graphene and highly oriented pyrolytic graphite (HOPG) on various magnetic and nonmagnetic substrates.

Understanding of the Magnetostriction in Fe-Ti Alloys by First-principles Calculations (2018–2019)

PROJECT ID 8J18AT004

PRINCIPAL INVESTIGATOR
Dr Dominik Legut

This project is focused on a theoretical identification of mechanisms that control the reduction and/or suppression of the thermal expansion of the dual-phase magnetostrictive Ti-based alloys. Concepts for controlling the thermal expansion may make use of a mixture of two phases, doping by an sp-element or using anti-ferromagnetic ordering in one of the phases in selected transition-metal (TM)-Ti alloys.

NEW

Physics of phononic interactions in solids for terahertz light generation (2019–2020)

PROJECT ID 8J19FR006

PRINCIPAL INVESTIGATOR
Dr Dominik Legut

New, compact solids for terahertz (THz) light generation open up new possibilities to apply terahertz radiation in wireless communication systems, security sensors and cameras, biomedicine, and spectroscopy. For subsequent application in THz frequencies ranging from 100 GHz up to 30 THz, compact high-performance coherent sources radiating under room temperature are indispensible. THz quantum cascade lasers (THz-QCL) offer a compact solution with high output performance. However, their high thermal dependence requires operation under cryogenic temperatures. On the other hand, fast development of quantum cascade lasers (QCL) in the mid-infrared spectral range allows much more efficient pumping of THz gas lasers, which is still insufficient for applications where compact THz lasers are required.

Grants of the Ministry of Education, Youth and Sports to support specific university research for the year 2019

Incoherent Effects in Multilayer Structures with Lateral Periodicity

PROJECT ID SP2019/151

PRINCIPAL INVESTIGATOR
Přemysl Ciompa

The project aims at elaborating the theory of incoherent effects in optical periodic systems. The existing methods for modelling incoherent effects in optical systems is based on averaging coherent fields, which are computationally intensive and are becoming more and more unfeasible for more complex 2D and 3D structures, thus hindering effective evaluation of experimental data and optimization of designed structues. Therefore, new and more efficient methods for modelling of incoherent effects need to be developed in order to conduct further research and optimization of complex optical components.

Advanced Modelling of Materials and Multiscale Modulated Nanostructures

PROJECT ID SP2019/110

PRINCIPAL INVESTIGATOR
Dr Lukáš Halagačka

The project is focused on studying new types of multiscale modulated surfaces, characterization of their optical properties, development and study of optical models of studied structures, and optimization of the prepared structures by numerical modelling. In addition, the project is focused on material design while respecting the typical range of operating conditions; mostly the effect of ambient temperature.

Quantification and Qualification Tool's Application to Dynamical Systems

PROJECT ID SP2019/125

PRINCIPAL INVESTIGATOR
Radek Halfar

The objective of the project is to study dynamical properties of systems, based on the state-of-the-art principle, motivated by real applications such as the Belousov-Zhabotinsky reaction, the Fenton-Karma model of a cardiac cell, and applications to real data of the Salomon supercomputer. For this purpose, some tools related to dynamical systems theory, such as recurrent matrices, approximation entropy, and the 0-1 test for chaos, will be used. Emphasis will be placed on correct identification of a problem and achieving new results by innovative approaches.

Extension of HPC platforms for executing scientific pipelines

PROJECT ID SP2019/108

PRINCIPAL INVESTIGATOR
Jan Křenek

The project is aimed at increasing possibilities to utilize HPC infrastructures using specialized services for remote execution of computational tasks. This extension will be implemented using the HPC-as-a-Service solution, special parallel programming models, and domain-specific programming languages. The extension will primarily be designed for problems in the fields such as traffic modelling, machine learning, and bioinformatics.

Internationalization of Doctoral Education in Molecular Physics II

PROJECT ID SP2019/162

PRINCIPAL INVESTIGATOR
Martin Mrovec

The project is focused on supporting internationalization of doctoral education in the field of molecular physics. Cooperation has been established with l'Université Toulouse III Paul Sabatier (UPS); ab initio calculations of potential hypersurfaces using the Molpro software and their representation using machine learning methods. Other research areas include solution of quantum physics problems using machine learning methods and testing and development of tools for application of machine learning methods.

Infrastructure Research and Development of HPC Libraries and Tools

PROJECT ID SP2019/59

PRINCIPAL INVESTIGATOR
Ondřej Vysocký

The project aims at development of existing tools developed at IT4Innovations in the Infrastructure Research Lab. The main focus is on efficient use of the infrastructure, which will be achieved as a result of optimization of libraries to increase performance as well as user comfort using a new web interface, and to enable visualization of scientific data using the most popular open-source 3D creation suite. The members of the project implementation team will be involved in implementation of new methods in the BEM4I library, implementation of a new I/O interface of the MERIC and RADAR tools, development of a new web interface of the ESPRESO library, and development of a new visualization tool based on the new version 2.8.

Using HPC to Solve Engineering Problems

PROJECT ID SP2019/97

PRINCIPAL INVESTIGATOR
Filip Zaoral

The project is dedicated to computational modelling of engineering problems in fields such as rotor system dynamics, topology optimization, and modelling of human thermoregulation using a biocybernetic approach. What the project topics share in common is that a finite element method and HPC resources are used to discretize a continuous continuum and to solve real problems, respectively. The main project tasks are as follows: (i) development of a program library core in MATLAB to model rotor systems discretized by 3D volume elements, (ii) development of a software package in MATLAB for topology optimization using the SIMP method, and (iii) implementation of Fiala passive and active models for human thermoregulation to a 3D human body geometry model.

Project supported by the Grant Agency of the Czech Republic

Novel Fuel Materials for Generation IV Nuclear Reactors(2017-2019)

PROJECT ID GA17-27790S

PRINCIPAL INVESTIGATOR
Dr Dominik Legut

The project is attempting to build an understanding of mechanical and thermodynamic properties of alloys designated for nuclear fuel for Generation IV nuclear reactors; alloys containing f-electrons, namely carbides and uranium, thorium, and plutonium tetrafluorides. Based on the ab-initio electronic structure calculations, magnetic, elastic, dynamic (phonons), and thermodynamic behaviour will be determined in (U/Th/Pu)-C systems. The main objective is to explain the thermal expansion of actinide carbides, and especially the negative thermal expansion observed in UC2 at the atomic level.

NEW

Space-time Boundary Element Methods for the Heat Equation (2019-2020)

PROJECT ID 19-29698L

PRINCIPAL INVESTIGATOR
Dr Michal Merta

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

Projects supported by the Technology Agency of the Czech Republic

Centre of Competence for Molecular Diagnostics and Personalized Medicine (2014-2019)

PROJECT ID TE02000058

PRINCIPAL INVESTIGATOR
Dr Branislav Jansík

The primary objective of the project is to apply and further foster the existing expert experience and to achieve a critical mass of participants and knowledge in research, development, manufacturing, protection of Intelectual Property, certification, technology transfer, and commercialization of in vitro diagnostics in order to create a market-oriented flexible national network of important institutions in the area of biomarkers and molecular diagnostics.

Parallelized Reaction Transport Model of Contamination Spread in Groundwater (2017-2019)

PROJECT ID TH02030840

PRINCIPAL INVESTIGATOR
Dr Michal Podhorányi

The objective of the project is to improve the possibilities of a potential risk analysis of environmental contamination due to the long-term radioactive substances spread around a deep radioactive waste repository via the surrounding rocky environment.

NEW

Personalized Medicine – Diagnostics and Therapy (2019-2020)

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 personalized diagnostic methods as well as drug candidates/drugs which would help specific groups of patients. The approach is highly interdisciplinary combining medicine, chemistry and biology, and 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 commercialized both by licensing and/or spin-off incorporation.

Projects supported by the Ministry of Industry and Trade

Intake and Discharge Objects of Pump and Turbine Stations (2018–2021)

PROJECT ID FV30104

PRINCIPAL INVESTIGATOR
Dr Tomáš Brzobohatý

The project objectives are as follows: 1. Development and verification of multiphase numerical computational model utilizing cavitation and free surface. 2. Experimental reseach of flow in model intake and discharge objects, creation of experimental results database for verification of numerical computational models. 3. Utilizing shape optimization for new design of pump and turbine stations, including intake and discharge objects.

NEW

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 to parts with the first part, i. e. research and development of the digital twin product, an asynchronous electric motor, being conducted at the Siemens branch, s.r.o. Elektromotory Frenštát.

Projects of Operational Programme Research, Development and Education

IT4Innovations National Supercomputing Center – Path to Exascale (2017–2021)

PROJECT ID EF16_013/0001791

PRINCIPAL INVESTIGATOR
Dr Branislav Jansík

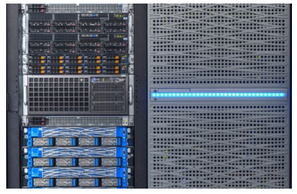
Some objectives of the project are to extend IT4Innovations in-house research in the field of modelling photonic and spin-photonic structures, design of progressive materials based on electronic structure calculations, and bioimage analysis using HPC. For the IT4Innovations infrastructure, in-house research is an important source of HPC expertise, which is reflected in the services provided by this infrastructure to its users.

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 AI 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 is based on 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.



Projects we are involved in

NEW

Optimization of Electrical Distribution System Operating Parameters Using Artificial Intelligence (2019–2021)

PROJECT ID TJ02000157

PRINCIPAL INVESTIGATOR
Jan Vysocký (ENET Centre, VSB-TUO)

The project goal is to create an optimization system and a strategy for optimizing the operation of the electrical distribution system (DS). The control optimization system will consist of a program and an interface. The program will set various DS elements to optimize the DS operation in many ways (i. e., operation with minimal cost, with maximum reliability, etc.). Optimal DS configuration will be achieved, for example, by changing network topology or controlling local active and reactive power sources. The interface will allow the proposed program to be included in the existing dispatching control structures of the DS. The optimization strategy will describe all the hardware and software innovations that need to be performed to maximize the DS management capabilities.

NEW

Contactless Detector for Partial Discharge Activity in Medium Overhead Voltage Powerlines (2019–2021)

PROJECT ID TJ02000031

PRINCIPAL INVESTIGATOR
Dr Jan Fulneček (ENET Centre, VSB-TUO)

The aim of this project is the development of an on-line insulation diagnostics tool for medium voltage overhead powerlines with covered conductors. A contactless sensor will be 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 discharges patterns in acquired signals will be 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 goal will be met by the end of the project duration.

NEW

National Centre for Energy (NCE) (2019–2020)

PROJECT ID TN01000007

PRINCIPAL INVESTIGATOR
Prof. Stanislav Mišák (ENET Centre, VSB-TUO)

The objective of the National Centre for Energy (NCE) is to stimulate long-term cooperation among the leading research organizations and major application entities in the power industry. Consequently, unique infrastructures and know-how of expert teams of the existing research centres will be shared through the implementation of joint applied research sub-projects. The research agenda of 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 decentralized sources of energy, use of alternative fuels to secure mineral resources independence and energy self-sufficiency of the Czech Republic, and power grids safety and security.

NEW

Energy System for Grids (2019–2023)

PROJECT ID TK02030039

PRINCIPAL INVESTIGATOR
Prof. Stanislav Mišák (ENET Centre, VSB-TUO)

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. 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 maximizing the exploitation of decentralized, 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 State Energy Conception within the 5-year implementation of the project.

NEW

Employment of Artificial Intelligence into an Emergency Call Reception (2019–2022)

PROJECT ID VI20192022169

PRINCIPAL INVESTIGATOR
Petr Berglowiec

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

International Grants

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

PROJECT ID
721865 (call no. H2020-MSCA-ITN-2016)

PRINCIPAL INVESTIGATOR
Prof. Tomáš Kozubek

The objective of this four-year long project is to educate researchers able to participate in interdisciplinary cooperation. The collaboration between industrial partners and research organizations will speed up development of key technologies for the development of turbines and their rapid commissioning in practice.

www.msca-expertise.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 will be implemented in the field of Customized Low Energy Computing for cyberphysical systems and the Internet of Things. The keypurpose of this initiative is to accelerate innovations in European industry. The initiative connects technical and application knowledge and experience, which helps small and medium-sized enterprises adopt advanced digital technologies more effectively and efficiently.

www.tetramax.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 is to contribute to efficient use of high performance computing by European small and medium-sized production companies and thus increase their competitiveness. This projects aims at optimization of production processes and productivity of companies using HPC-based modelling and simulation as well as cloud services.

www.cloudifacturing.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, is to develop new methods allowing solution of complex engineering problems using numerical simulations on future exascale systems. Within the project, new computing methods and software tools will be developed for solving simulations of aerodynamics for optimizing geometrically complex civil engineering structures.

IT4Innovations will participate in deploying the Hyperloom and COMPSs tools using high performance computing systems, their configuration, and optimization. Our participation also includes testing of robust algorithms for shape optimization of wind-loaded structures.

www.exaqute.eu

POP2 – Performance Optimisation and Productivity 2 (2018–2021)

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 analysis of parallel applications, identification of erroneous parts of codes, and recommendations of optimization methods resulting in increased performance and better scalability of a given application.

https://pop-coe.eu/

NEW

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

PROJECT ID
825532 (H2020-ICT-2018-2020)

PRINCIPAL INVESTIGATOR
Dr Jan Martinovič

The objective of the project of which IT4Innovations is the Coordinator is 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 projects will be demonstrated via three pilot tests suitable for industrial fields such as aerospace, weather and climate, and earthquakes and tsunami.

https://lexis-project.eu

NEW

OPENQKD – Open European Quantum Key Distribution Testbed (2019–2022)

PROJECT ID
857156 (H2020-SU-ICT-2018-2020)

PRINCIPAL INVESTIGATOR
Prof. Miroslav Vozňák

The project aims at establishing a testbed for a highly-secure network using principles of quantum mechanicsforkeydistribution.Ithasbeenthe 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 Networing Center (PSNC). The second is participation in the development and implementation of key management. The last is a simulation of QKD use cases of all partners in the project, and also an improvement of an open-source QKD simulator, which is being developed in Ostrava. For the simulations, the resources of the IT4Innovations National Supercomputing Center are used.

https://openqkd.eu/

Collaboration with the Commercial Sector

Collaboration with the commercial sector is implemented at IT4Innovations mainly in the form of contract research. Our contract research in 2019 included collaboration with these companies:

- Bayncore Labs Limited
- Continental Powertrain Czech Republic s.r.o.
- Glass Service a.s.
- ING corporation, spol. s r.o.
- K2 atmitec s.r.o.
- Ministry of Industry and Trade
- National Cyber and Information Security Agency
- Siemens s.r.o.
- The German Aerospace Center

EDUCATIONAL AND TRAINING ACTIVITIES

Study Programs

IT4Innovations together with the Faculty of Electrical Engineering and Computer Science of VSB-TUO run the Computational Sciences PhD study program. Being unique within the Czech Republic, this program was opened in the 2015-2016 academic year, and is focused on use of HPC, HPDA, and AI in science and industry. At the end of the year 2019, there were 19 students studying within this programme. The Computational Sciences PhD study program is part of the MathInHPC Doctoral School, bringing together leading Czech workplaces focused on research in the field of HPC methods and their application. Its students thus have an opportunity to get in touch with prominent experts from the Doctoral School partner institutions such as the Faculty of Mathematics and Physics of CU and the Institute of Mathematics of the CAS.

IT4Innovations is also strongly engaged in teaching within the Computational and Applied Mathematics MSc study program, 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 specialization.

Educational Activities

IT4Innovations supports the scientific community as well as its users by organizing high-quality courses, tutorials, workshops, and other educational events. The primary objective of these activities is to broadly enhance 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 2019, IT4Innovations organized 8 educational activities attended by 249 participants.

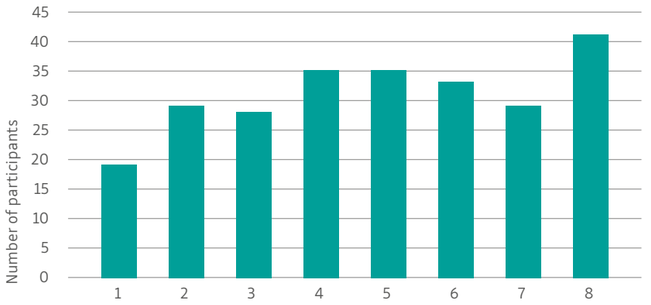
Having been awarded **PRACE TRAINING CENTER** (PTC) status in 2017, IT4Innovations organized six courses under the auspices of PRACE in 2019. Among others, these courses included:

- **PARALLEL VISUALIZATION OF SCIENTIFIC DATA USING BLENDER** (Petr Strakoš, Milan Jaroš, Alena Ješko), focused on hands-on training of basic operations of the popular open-source 3D creation suite - Blender.
- **DATA SCIENCE WITH R AND PYTHON** (Tomáš Martinovič, Stanislav Böhm), where participants obtained basic as well as advanced knowledge required for analysis and visualization of scientific data using the R and Python programming languages.

Having the status of **NVIDIA Deep Learning Institute Ambassador**, IT4Innovations also offered (in 2019) practical courses for developers and researchers wishing to solve complex problems using deep learning. These courses ranked among the most successful ones.

- **GET STARTED WITH INTEL AND NVIDIA ARTIFICIAL INTELLIGENCE TECHNOLOGIES** (Georg Zitzlsberger, Stephen Blair-Chappell). The participants of this two-day course learnt about the basics of Machine Learning for efficient work on CPU (i.e. Intel Architecture). They also had an opportunity to use the Deep Learning training model in practice and deploy it in the target Intel Movidius Compute Stick application and run it independently.
- **FUNDAMENTALS OF DEEP LEARNING FOR COMPUTER VISION** (Georg Zitzlsberger). In this course focused on Deep Learning basics using neural network training, the participants learnt about the implementation of workflows, the use of strategies for enhancing performance and capabilities of deep learning using neural networks, and applied this method in practice.

Educational activities in 2019



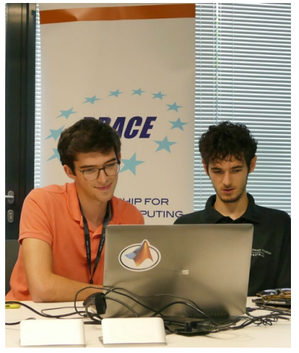
1. Developing efficient HPC applications for the latest CPU architectures with C++ and Fortran (PTC course)
2. Parallel visualization of scientific data using Blender (PTC course)
3. Parallel visualization of scientific data using Blender
4. Data science with R and Python (PTC course)
5. Fundamentals of Deep Learning for Computer Vision (PTC course)
6. Fundamentals of Deep Learning for Computer Vision
7. Productivity tools for High Performance Computing (PTC course)
8. Get Started with Intel and NVIDIA Artificial Intelligence Technologies (PTC course)

PRACE Summer of HPC

Already for the 7th time, the Partnership for Advanced Computing in Europe (PRACE) allowed students to participate in a summer internship taking place in supercomputing centres all over Europe. This time, the opportunity was given to 25 students across 11 host organizations. IT4Innovations hosted two of them.

Within the PRACE Summer of HPC, David Izquierdo, a BSc. student of aerospace engineering at Carlos III University of Madrid, worked on the project entitled Analysis of CFD simulations of Aerodynamics of Cars - Formula Student. His mentor was Tomáš Brzobohatý from the Parallel Algorithms Research Lab.

Pablo Lluch Romero, a BSc. student of artificial intelligence and software engineering in Edinburgh, worked on the project entitled Emotion Recognition using Deep Neural Network. His mentor was Georg Zitzlsberger from the Advanced Data and Simulation Lab. For his project, Pablo Lluch Romero received the Ambassador Award – PRACE Summer of HPC 2019.



Educational Projects

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
(call no. 02_16_018)

PRINCIPAL INVESTIGATOR
Doc. 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 modernize and internationalize one of the doctoral programs 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).

Technique for the Future (2016–2020)

PROJECT ID
CZ.02.2.69/0.0/0.0/16_015/0002338
(call no. 02_16_015)

IT4INNOVATIONS PROJECT SPECIALIST
Doc. René Kalus

PThe project of VSB – Technical University of Ostrava "Technique for the Future" aims at creating or modifying strategic study programmes so that they reflect the demands of employers and prepare students for successful entry into the labor market. The project focuses on the introduction of progressive teaching methods using state-of-the-art technical equipment, collaboration with companies and graduates, strengthening the internationalism of the university, improving work with students with various handicaps, improving the quality system and management of the university, and promoting student entrepreneurship.

Science without Borders (2018–2020)

PROJECT ID
CZ.02.2.69/0.0/0.0/16_027/0008463
(call no. 02_16_027)

IT4INNOVATIONS PROJECT COORDINATOR Prof. Tomáš Kozubek

The objective of the VSB – Technical University of Ostrava project is to implement 43 international mobilities, Projects which will lead to professional development, enhancement of qualification and other skills of both junior and senior researchers, thereby acquiring and transferring of experience abroad as well as ensuring foreign experts at VSB – Technical University of Ostrava. Mobilities shall allow participation in international chains of scientific laboratories and academic institutions primarily, although not exclusively, within the European Research Area (ERA), an increase in the intensity of establishing international contacts, and involvement in international R&D initiatives and projects.

NEW

Techniques for the future 2.0 (2019–2022)

PROJECT ID
CZ.02.2.69/0.0/0.0/18_058/0010212
(call no. 02_18_058)

IT4INNOVATIONS PROJECT SPECIALIST
Doc. 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 internationalization of the university and ties between the university and its graduates. It implements methods for increasing 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 the VSB-TUO educational activities for 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.

International Visegrad Fund project

Superheroes 4 Science (2018–2020)

PROJECT ID 21820033

PRINCIPAL INVESTIGATOR
Karina Pešatová, MBA

A joint project of partners from the Visegrad Four (IT4Innovations National Supercomputing Center, the Governmental Information Technology Development Agency of Hungary, the Computing Center of the Centre of Operations of the Slovak Academy of Sciences, Poznań Supercomputing and Networking Center – the Institute of Bioorganic Chemistry of the Polish Academy of Sciences) aims at explaining attractively the importance of supercomputers and their use, which has a positive impact on the everyday life of people. Each project partner provides information about their national supercomputing infrastructure and dedicates substantial effort to popularisation activities focused on increasing awareness of supercomputing, its ever-increasing importance for society, and justification of investments therein. The understanding of both scientific topics and supercomputing is not easy for non-experts at all. In order to make communication of the relatively complex content easier, the resulting materials will be adapted to different target groups based on the age, level of education as well as qualification. The objective of the project is to not only educate the wider public, but to also inspire the younger generation in Visegrad countries to enrol for scientifically and technologically oriented study programmes.

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

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MINISTRY OF EDUCATION, YOUTH AND SPORTS

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