NEWSLETTER Q3/2020

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

IN BRIEF

BARBORA CELEBRATED ITS 1ST BIRTHDAY

Our Barbora supercomputer celebrated its 1st birthday in early October. Within a year, its 37,542,601 core hours were distributed among 114 projects.

More information about Barbora HERE

EUROHPC JU LAUNCHED ITS WEBSITE

EuroHPC JU, which is financially involved in the procurement of our new supercomputer, introduced Anders Dam Jensen, the new Managing Director. It also launched a website that brings information about HPC activities in Europe.

EuroHPC Joint Undertaking

eurohpc-ju.europa.eu

TERATEC 2020 DIGITAL FORUM

Our colleagues from the LEXIS and ExaQUte projects were virtually present at the Teratec 2020 Digital Forum held on 13th and 14th October. The forum, which brings together the best international experts in the field of HPC simulations and Big Data, took an online form and offered registered users a series of workshops, online meetings, and even the opportunity to create a virtual booth for their project.

More about Digital Teratec Forum HERE

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IN BRIEF

HIGH-PERFORMANCE QUANTUM CALCULATIONS ARE WITHIN REACH

The LUMI consortium, a member of which is also IT4Innovations, has brought together high-tech centres across Europe not only for traditional HPC but also in the context of quantum computer technologies. Are you interested in what is new in this field and what direction quantum computing technologies are taking? Then be sure not to miss an article on the subject.

For the article, read HERE

LUMI SUPERCOMPUTER TO BE DELIVERED BY HPE

IT4Innovations is a member of the LUMI consortium that will launch the pre-exascale LUMI supercomputer with a theoretical peak performance of 552 PFlop/s in 2021! This, like our supercomputer with the working name EURO_IT4I, will be supplied by the HPE company. The LUMI supercomputer will be located in Finland, but institutions from the Czech Republic will also have access to it. With its extraordinary computing power, LUMI will solve even the most computationally intensive research challenges of today.

For more details, see HERE

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IT4INNOVATIONS ONE STEP CLOSER TO LAUNCHING THE MOST POWERFUL SUPERCOMPUTER IN THE CZECH REPUBLIC

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IT4Innovations one step closer to launching the most powerful supercomputer in the Czech Republic

At the beginning of October, an agreement was signed to procure a new supercomputer, which will be launched at IT4Innovations in the first half of 2021. The supercomputer, which will serve not only academia but also public institutions and industry, will be delivered by Hewlett Packard Enterprise.

In the spring of 2019, IT4Innovations National Supercomputing Center achieved success with their project titled IT4Innovations Centre for European Science and Industry in a pan-European competition to host a European petascale supercomputing system, which will be built under the EuroHPC JU. A public procurement procedure to select the economic operator to supply the system was commenced, from which Hewlett Packard Enterprise emerged as the winner, becoming the supplier of the system with a theoretical peak performance of 15.2 PFlop/s.

The cost of the procured system will total almost EUR 15 million, 35%, i.e. EUR 5.13 million, of which will be paid by the EuroHPC JU. The remaining costs amounting to EUR 9.73 million will be funded using the resources of the European Structural and Investment Funds through the Operational Programme Research, Development and Education (OP RDE). The installation and launching of this unique computing system are planned for the first quarter of 2021, and its service to science, industry, and society is planned to be provided until 2025. Its total operating costs between 2021 and 2025 are estimated at EUR 14 million.

"IT4Innovations has long established itself as a leading research, development, and innovation centre in the field of high-performance computing, data analysis, and artificial intelligence with excellent reputation across Europe. I believe that by procuring this system, the position of IT4Innovations as a major European supercomputing centre will be further consolidated, while at the same time bringing our university interesting projects from both its in-house and external users from academia and industry," said Vaclav Snasel, the Rector of VSB – Technical University of Ostrava.

Anders Dam Jensen, the Executive Director of the EuroHPC JU added: *"This new world-class supercomputer, located in the Czech Republic will benefit Europe as a whole and will bring us one step closer to our ambition of making Europe a global leader in high performance computing. Its computing power will be accessible to European public, scientific and industrial users wherever they are in Europe, for instance to improve weather predictions, develop greener energy infrastructures or adapt therapies to the specific needs of a patient."*

"I must admit that I am proud of the fact that through the supply of technology developed by our company, we can contribute to the Czech Republic's further development in progressive areas such as machine learning, artificial intelligence, and advanced big data analysis," said Jan Kamenicek, Managing Director of Hewlett Packard Enterprise for the Czech Republic. *"The proposed solution is built on HPE's unique technologies in combination with those developed by SGI and Cray, whose acquisitions have enabled HPE to expand massively on the market and develop a portfolio of products and services in the field of high-performance computing and supercomputing. The implementation of this project will also allow us to further strengthen our top local team, which is both dedicated to the field of supercomputing and unique in the context of Central and Eastern Europe,"* adds Kamenicek.

"Our users' demands for computational resources are growing every year, and we have not been able to fully meet them anymore. This brand-new supercomputer is designed to fully cover user requirements in solving complex scientific and industrial problems involving, for example, classical numerical simulations, large-scale data analysis, and the use of artificial intelligence," adds Vít Vondrak, the Managing Director of IT4Innovations National Supercomputing Center.

The supercomputer with working title EURO_IT4I will achieve a theoretical peak performance of 15.2 PFlop/s, thus becoming the most powerful supercomputer in the Czech Republic with an ambition to rank 10th in Europe and 50th in the world. It will thus exceed the performance of Salomon, the most powerful supercomputer at IT4Inno-

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vations to date, with a theoretical peak performance of 2 PFlop/s, reached many times. It is certainly worth noting that the accelerated part of the supercomputer, which will be made up of HPE Apollo 6500 servers with a total of 560 NVIDIA A100 Tensor Core GPUs that provide, among other things, a theoretical peak performance for artificial intelligence calculations of up to 150 PFlop/s. The supercomputer will be interconnected with NVIDIA Mellanox HDR 200Gb/s InfiniBand, delivering extremely low latency, and smart in-network computing acceleration engines. With NVIDIA GPU acceleration and smart InfiniBand offload engines, the new system will be perfectly prepared to handle very demanding, computationally intensive tasks in the fields of machine learning and artificial intelligence, which are delivering scientific breakthroughs across the globe.

The procurement of the EuroHPC supercomputer is funded by the OP RDE project entitled IT4Innovations national supercomputing center – path to exascale, project ID: CZ.02.1.01/0.0/0.0/16_013/0001791. The procurement and operation of the EuroHPC supercomputer is jointly funded by EuroHPC JU, through the European Union Connecting Europe Facility and the Horizon 2020 research and innovation programme, as well as the Czech Republic.

TECHNICAL DATA

- More than 100,000 CPU cores and 250 TB of RAM,
- More than 3.8 million CUDA cores / 240,000 tensor cores of NVIDIA A100 Tensor Core GPU accelerators with a total of 22.4 TB of superfast HBM2 memory,
- 15.2 PFlop/s total theoretical computing power,
- Fast disk capacity with a capacity of 1 TB/s.

THE SUPERCOMPUTER WILL CONSIST OF 6 MAIN PARTS

- A universal part for standard numerical simulations, which will consist of approximately 720 computer servers with a theoretical peak performance of 3.8 PFlop/s,
- An accelerated part with 70 servers and each of them being equipped with 8 GPU accelerators providing a performance of 11 PFlop/s for standard HPC simulations and up to 150 PFlop/s for artificial intelligence computations,
- A part designated for large dataset processing that will provide a shared memory of as high as 24 TB, and a performance of 74 TFlop/s,
- 36 servers with a performance of 131 TFlop/s will be dedicated for providing cloud services,
- A high-speed network to connect all parts as well as individual servers at a speed of up to 200 Gb/s,
- Data storages that will provide space for more than 1 PB of user data and will also include high-speed data storage with a speed of 1 TB/s for simulations as well as computations in the fields of advanced data analysis and artificial intelligence.

EUROPEAN UNION
European Structural and Investment Funds
Operational Programme Research,
Development and Education

MINISTRY OF EDUCATION, YOUTH AND SPORTS

EuroHPC
Joint Undertaking

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EURO

IT4INNOVATIONS BECOMES THE NATIONAL COMPETENCE CENTRE IN HPC

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IT4Innovations becomes the National Competence Centre in HPC

On 1st September, IT4Innovations joined the EuroCC project, which aims to share knowledge in high-performance computing (HPC) across Europe and enhance the EU's technological autonomy and competitiveness. In the Czech Republic, a national competence centre for HPC and supporting activities in this field focused on industry, public administration, and academia will be established and introduced, respectively, within the EuroCC project.

Following the European Commission's priority given to the widespread use of HPC and related disciplines such as data analysis and processing and artificial intelligence, the EuroHPC JU has approved funding for a project to create a pan-European network of national HPC Competence Centres. The project is called EuroCC and the role of the National HPC Centre of Competence for the Czech Republic is held by IT4Innovations National Supercomputer Center at VSB – Technical University of Ostrava.

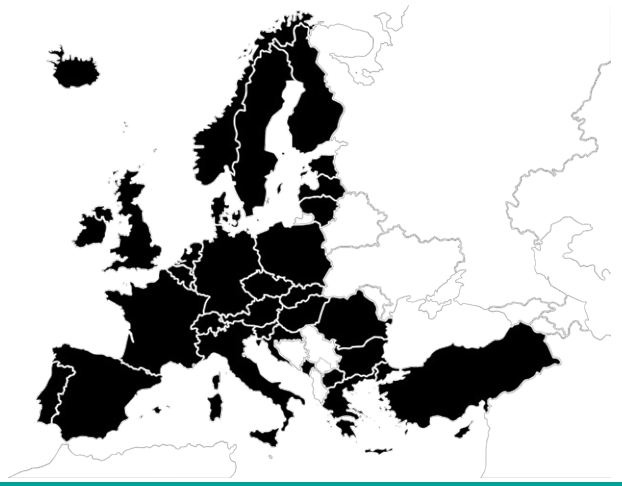
"The EuroCC project aims at establishing a pan-European network of National HPC Competence Centres to increase HPC knowledge. These centres will support academia, public administration, and industry, particularly small and medium--sized enterprises, and promote the use of available knowledge, expertise, and HPC resources in Europe to them," explains Tomas Karasek, the project coordinator for the Czech Republic from IT4Innovations National Supercomputing Center at VSB-TUO.

At the same time, the CASTIEL project, which seeks to exchange expertise across the EuroCC network, has also been launched. For the future, the EuroCC project will offer expert support, courses, trainings, and workshops through the Competence Centres. In addition, the project will provide mentoring not only to enable a better understanding and addressing the specific needs of industrial users of HPC technologies but also to assist SMEs in making investment decisions in HPC technologies and resources, all via the national competence centres and international meetings.

This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 951732. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Germany, Bulgaria, Austria, Croatia, Cyprus, the Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, the United Kingdom, France, the Netherlands, Belgium, Luxembourg, Slovakia, Norway, Switzerland, Turkey, Republic of North Macedonia, Iceland, Montenegro.

EUROCC PROJECT

- **brings together 33 European countries,**
- **total budget amounting to EUR 57 million,**
- **the first phase of the project will last for two years,**
- **start of the EuroCC Project on September 1, 2020.**



www.eurocc-project.eu

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EVALUATION OF THE 19TH OPEN ACCESS GRANT COMPETITION

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Evaluation of the 19th Open Access Grant Competition

In the 19th Open Access Grant Competition interested users applied for more than 90,5 million core hours. The required resources exceeded the capacity by 24%. With respect to high demand in the computational resources, the allocation committee decided to decrease the initial allocation for each individual project. In this Open Access Grant Competition, the allocation committee have thus distributed 73 million core hours across 57 successful projects, with 10 of them being multi-year projects.

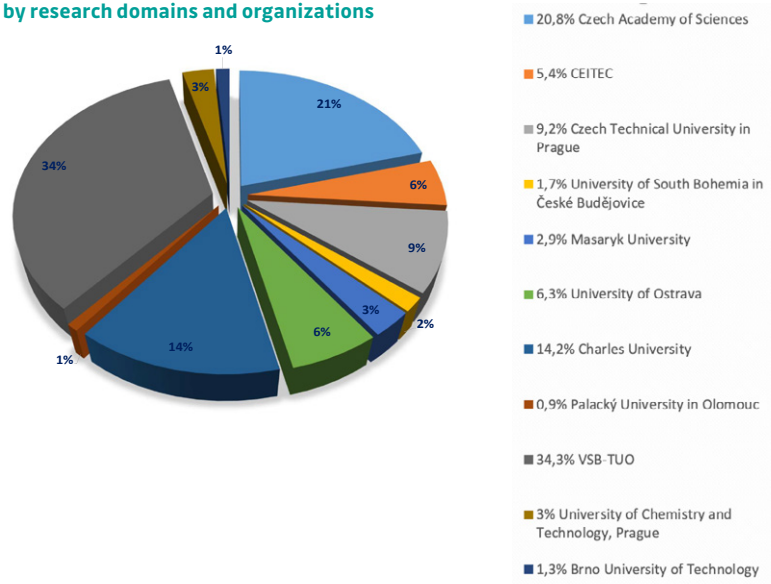
Most of the core hours, specifically 20.5 million (i.e., 34% of the total distributed computational resources), were awarded to researchers from VSB – Technical University of Ostrava for 19 projects. Institutes of the Czech Academy of Sciences were awarded more than 12.5 million core hours (i.e., 21% of the total distributed computational resources) for 12 projects, and Charles University in Prague was awarded 8.5 million core hours (i.e. 14% of the total distributed computational resources) for 6 projects.

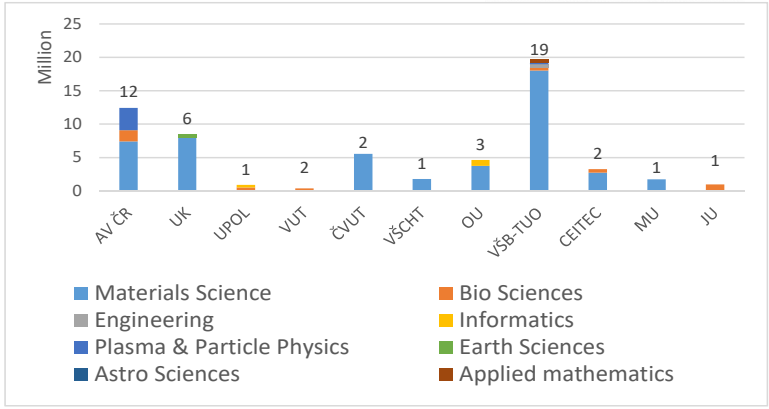
Other institutions awarded the computational resources for implementing their research projects in the 19th Open Access Grant Competition include CTU in Prague, the University of Ostrava, CEITEC, Brno University of Technology, the University of Chemistry and Technology in Prague, Palacký University in Olomouc, Masaryk University, and University of South Bohemia in České Budějovice.

Allocation of computational resources in the 19th Open Access Grant Competition by research domains and organizations

Allocation of more than 1 million core hours was awarded to 18 projects of researchers from Charles University in Prague, the Czech Technical University in Prague, the Czech Academy of Sciences, the University of Chemistry and Technology in Prague, Masaryk University, CEITEC, the University of Ostrava, Masaryk University in Brno, and VSB – Technical University of Ostrava. The first three most successful projects were awarded a total amount of 18 million core hours. More than 9 million core hours were awarded to Dominik Legut from IT4Innovations for his project "Ultrastrong Graphene-Transition Metal Carbide and Nitride Heterostructures: A Road to Superhard Materials". and Mojmir Sob from CEITEC for his project entitled "The Entropy--driven Segregation of Impurities at Grain Boundaries", respectively. The third highest allocation was awarded to Prof. Pavel Hobza from the Institute of Organic and Inorganic Chemistry of the CAS for his project entitled "In Silico Drug Design". Pablo Nieves from IT4Innovations can use more than 5 million core hours for his project "Magneto-AELAS: Software for the High-throughput Calculation of Magnetostrictive Coefficients" and the third highest allocation was received by Martin Zeleny from Charles University with his project "Design of a New Smart Material with Magnetic Shape Memory Effect".

Allocation of computational resources in the 19th Open Access Grant Competition by research domains and organizations





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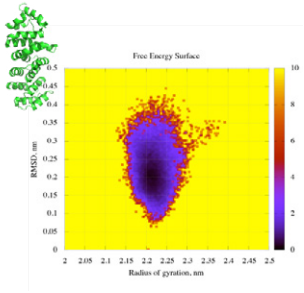
LET US INTRODUCE SOME OF THE AWARDED PROJECTS:

Dr. Olena Mokshyna
Institute of Molecular and Translational Medicine, Palacky University in Olomouc

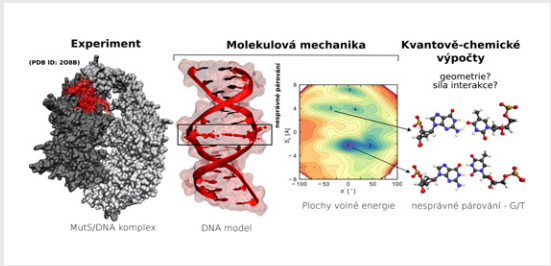
SEARCH FOR NEW ANTICANCER COMPOUNDS AND INVESTIGATION THEIR MECHANISM OF ACTION



The development of novel anticancer agents is a long and complicated process, which involves an investigation of many potential targets for such therapies. In this project we are going to address several of such targets. Bystin is a compact protein promoting human cancer cell growth. Despite bystin being a promising target for anticancer drugs and drugs against Blackfan anemia, no site of binding was previously identified. Olena Mokshyna, who was awarded 510 000 core hours for her project, found that bystin has two primary shallow binding sites. Exploring the mechanisms of binding of promising drug-like compounds, she was able to establish stable binding poses for most of the ligands and distinguish two main groups of ligands with varying activity. Her project aims to further explore bystin dynamics using enhanced sampling methods and perform free energy calculations of ligand-protein systems. These methods are used with emphasis on metadynamics simulations, which would allow to explore the ligands' mechanism of actions in silico. The second target protein is CYP2w1. The uniqueness of CYP2w1 consists in the fact that it is mostly expressed in tumor cells rather than in healthy tissues. This feature makes it a potential target for selective anticancer agents. There are currently a few compounds known, which not only selectively bind to the metabolic site of the protein but also turn to a cytotoxic compound, thus destroying a cancer cell, but not damaging the healthy tissues. Olena Mokshyna aims to perform virtual screening to select compounds with a similar mode of action for further experimental testing. The results of her project will facilitate development of anticancer drugs and medication to treat Diamond-Blackfan anemia.

Dr Petr Kulhanek
CEITEC, Masaryk University

QUANTUM MECHANICAL MODELING OF MISMATCHED DNA



Deoxiribonucleic acid (DNA)double helix is composed of two complementary strands, which are held together by Watson-Crick base pairing. Base-pairing mismatches can result in the development of inherited genetic diseases, cancer, and aging. Therefore, organisms developed several ways how to detect and repair these base-pairing errors and thus keep the integrity of genetic information for next generations. One of them is the mismatch repair pathway (MMR), in which the MutS enzyme detects mismatches and once found, it triggers a cascade of processes leading towards their repair. Petr Kulhanek and his research team tried to decipher how MutS can effectively detect base-pairing mismatches. In order to do so, they applied molecular mechanics and dynamics methods based on simplified physical description. This, at the cost of lower accuracy, makes it possible to study large biomolecular systems. Petr Kulhánek will use the awarded 532 000 core hours for quantum-chemical calculations to validate accuracy of the results achieved in previous studies. In this way, he will not only obtain information on the quality of the simplified physical description but also more detailed information about individual interactions in non-complementary base pairing and their relevance to MutS enzyme recognition. The obtained data is important for future rational design of chemical substances suitable in anti-cancer therapy, which will target damaged DNA.

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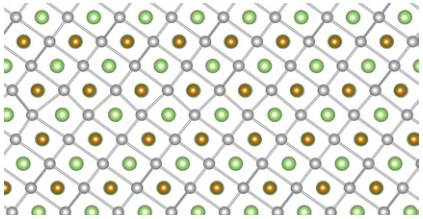
Dr Martin Zeleny
Faculty of Mathematics and Physics, Charles University in Prague

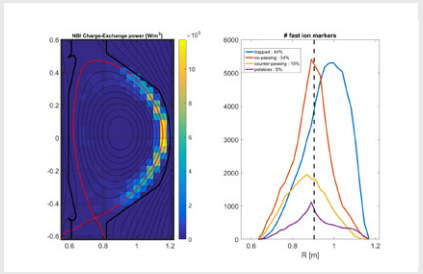
DESIGN OF A NEW SMART MATERIAL WITH MAGNETIC SHAPE MEMORY EFFECT



Magnetic shape memory (MSM) alloys have a large application potential in actuators, sensors, energy harvesters, and magnetic refrigeration systems thanks to the extraordinary properties of their multiferroic martensite structure. The macroscopic deformation of such materials in an external magnetic field is caused by the motion of highly mobile twin boundaries in combination with high magnetic anisotropy. However, operating temperatures of currently used materials are too low for engineering applications, which is caused by their low transformation temperatures between austenite and martensite. Within the OP RDE MATFUN project, which was awarded more than 4.1 million core hours in the first period, Martin Zeleny will search for new materials with a high application potential that combine the stability of martensitic phase up to high temperature with its high magnetic anisotropy and low twining stress necessary for motion of twin boundaries, which are also necessary prerequisites of a successful MSM alloy development. Such alloys will in turn enable the miniaturisation and development of new devices in robotics, automotive, aerospace, and biomedical industries. In addition to finding new candidates for experimental preparation, Martin Zeleny will also investigate in depth the basic aspects of the multiferroic behaviour of alloys with magnetic shape memory, such as the physical origin of the martensitic transformation or the mobility of twin boundaries.

Dr Fabien Jaulmes
Institute of Plasma Physics of the Czech Academy of Sciences

COMPUTATIONAL MODELLING OF FAST ION ORBITS IN TOKAMAK



Nuclear fusion technology might enable us to generate energy without releasing large amounts of greenhouse gases into the atmosphere or leaving behind us long lived radioactive waste. Among the approaches to fusion, tokamak seems to be the most promising one. The concept involves the use of magnetic fields to confine plasma hot enough to sustain fusion within itself. Within the international ITER project, a new tokamak is being built in Southern France. If successful, the device would be the first one of its kind to produce net energy. COMPASS is a small tokamak located in Prague, Czech Republic. It allows scientific investigation of various physics issues related to the operation of the future ITER. Fabien Jaulmes and his team was awarded more than 1.7 million core hours for his project focused on the study and modelling of narrow band imaging-born particle (NBI) behaviour, which might have impact on the future design of the system and its integration in COMPASS as wel as in the planned upgrade of the machine in 2022. The project aims at achieving better scientific understanding of tokamak nuclear power stations as well as cheaper and more sustainable power generation on larger scale. Having high potential impact on future reactor maintenance costs, this study aims to optimise heating systems.

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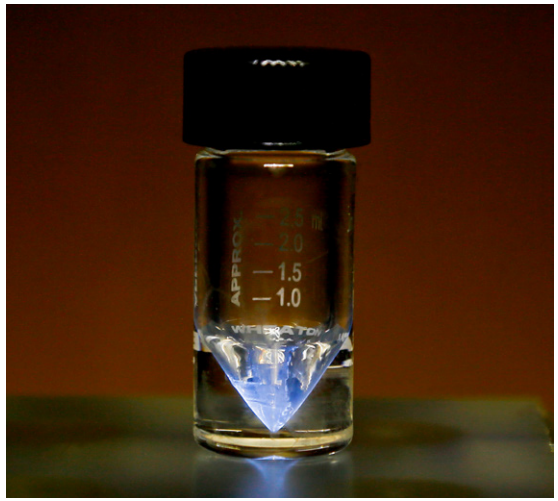
Lukas Kyvala
IT4Innovations, VSB-TUO

THERMODYNAMICS OF ACTINIUM METAL

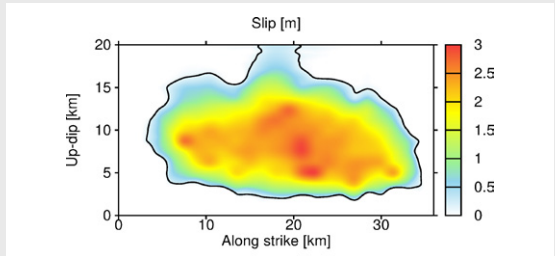
The half-life of the most stable actinium isotope is only 21.77 years. Therefore, its concentration in nature is significantly low. Were it not for one of the products of the decay of thorium and uranium, it would have long since disappeared from Earth. Due to its high radioactivity, only a few experiments on metal actinium were done and actinium remains as one of the least explored naturally occurring elements. Even the basic property as lattice constant has been subject of discussion for many years and its unusually small value has not been fully elucidated. Lukas Kyvala will use the awarded computational resources (272 000 core hours) to analyse physical properties of actinium, its stability under different temperatures, and the relativistic effects as actinium, due to its high radioactivity (150 times higher than in the case of radium) has become a preferred element in radiotherapy. Study of actinium might not only help understand the physics of actinoids but also enable the obtained knowledge to be utilized in its applications such as the source of neutrons and geochemical indicator for deep circulation of sea water. Moreover, its ability to deliver stable amounts of heat is suitable for generating electricity in space where solar power is not available (i.e., for missions on the dark side of the moon).



Dr Lubica Valentova
Faculty of Mathematics and Physics, Charles University in Prague

RUPTURE PARAMETERS OF DYNAMIC SOURCE MODELS COMPATIBLE WITH EMPIRICAL GROUND MOTIONS

Within the project awarded 481 000 core hours, the seismology team from the Department of Geophysics at the Faculty of Mathematics and Physics of Charles University in Prague will focus on the study of earthquake source model parameters that control the rupture propagation process on a fault. Based on the random sampling method, they will generate a large number of rupture propagation simulations (up to several ten thousand). However, not all such synthetic earthquakes correspond to real phenomena. Therefore, statistically, only those simulations that generate strong ground motions agreeing with observations from a large number of real earthquakes, i.e. an empirical model, are accepted into the database. The result will take the form of a large database of earthquake scenarios (several thousand) with varying magnitudes and varying complexities of rupture propagation. These phenomena arise from the determined laws of physics for processes at the fault, while at the same time arousing realistic ground movements. Due to the complexity of this synthetic database and lack of observation errors, characteristics such as rupture duration, size of the ruptured area, stress drop, and energy budget are compared with their real counterparts determined from actual phenomena in further analysis. The key focus in this project includes the study of obtained parameters acting in the friction law (their variance and potential correlations), which are not generally accessible for real events and which have significant impact on the resulting ground motions. Thus, studying a seismic source using numerical simulations may also be useful for assessing the effects of earthquakes and seismic hazards.



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WE HAVE BECOME A PARTNER OF THE CENTRE FOR ENERGY AND ENVIRONMENTAL TECHNOLOGIES

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We have become a partner of the Centre for Energy and Environmental Technologies

IT4Innovations cooperates with the ENET centre, which is part of VSB – Technical University of Ostrava, in the Centre for Energy and Environmental Technologies (CEET) project. The project is supported by the Technology Agency of the Czech Republic, which financially supports research and innovation.

The CEET project aims to find solutions for the efficient transformation of alternative fuels, wastes and by-products into recovered chemicals and useful forms of energy. However, CEET also addresses their storage and efficient use, with the support of the digital twin's most modern methods and technologies, in line with the principles of the circular economy. Launched in August of this year under the command of Professor Stanislav Misak of the ENET VSB-TUO Centre, the project is scheduled for five years. Besides VSB-TUO (ENET and IT4Innovations), other participants in the project are the Institute of Plasma Physics of the CAS, v.v.i. and the SMOLO a.s., APT, spol. s r.o. and ABB s.r.o. companies. IT4Innovations is responsible for creating the CEET digital twin. The development of this complex energy system will allow virtual modelling of selected operational states of the entire technology chain. This is composed of alternative fuel processing equipment and equipment for separation, filtration, and the use of hydrogen from those processes (e.g., in hydrogen car stations). The selected technology chain will be mathematically defined into a virtual twin for selected operating states, and the virtual model will include a building information model (BIM) for the entire test polygon.

"A digital twin is a software (virtual) copy of a real system that allows you to remotely monitor and evaluate the state of a real object. But the digital copy is not just a duplicate of reality, for it contains, thanks to the dreamers, measured data about the object and its condition. Therefore, thanks to the digital twin, different scenarios can be modelled and evaluated, finding vulnerabilities, anomalies, and finding optimal solutions that can then be applied to control a real object. The digital twin uses, among other things, sensors, data networks, and modern prediction algorithms, including artificial intelligence methods," explains Pavel Praks from the Advanced Data Analysis and Simulation Lab of IT4Innovations. As part of the development of the CEET's digital twin, we are testing the artificial intelligence methods of the Austrian SymReg.at project. We also analyse automated machine learning (AutoML) methods. IT4Innovations has a large number of machine learning methods at its disposal, but the question arises as to which method to use and how to properly set its parameters. Automated machine learning methods help facilitate the selection of machine learning algorithms, recommend appropriate parameter settings as well as data preprocessing, and improve the ability to detect complex patterns in big data (http://automl.info/automl). The advantage is to refine prediction models, the disadvantage, on the other hand, is the high computational power. However, calculations can be speeded up by using IT4Innovations supercomputers able to run the method tests in parallel.

WHAT IS THE DIGITAL TWIN?

The digital twin's roots date back to the 1970s, when an oxygen tank exploded on the Apollo 13 mission, endangering the mission and crew. However, NASA had a faithful spacecraft mock-up, simulating both the malfunction and the subsequent solution used to repair the spacecraft. Nowadays, they use computer modelling instead of mock-ups. Similarly, a digital twin of the production process is being created. Sensors monitor the status of the device, and data is transmitted by the computer network and stored in the database. Thanks to the mathematical model and information on the history and current state of the device, the entire manufacturing process can be simulated by a computer, including wear and tear on the components, and design, among other things, an optimal maintenance strategy.

The project, grant no. TK03020027 CEET – Centre for Energy and Environmental Technologies is co-funded by the Technology Agency of the Czech Republic under the THETA Programme for Applied Research, Experimental Development, and Innovation

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HPC PLATFORMS FOR SCIENTIFIC WORKFLOW EXECUTION

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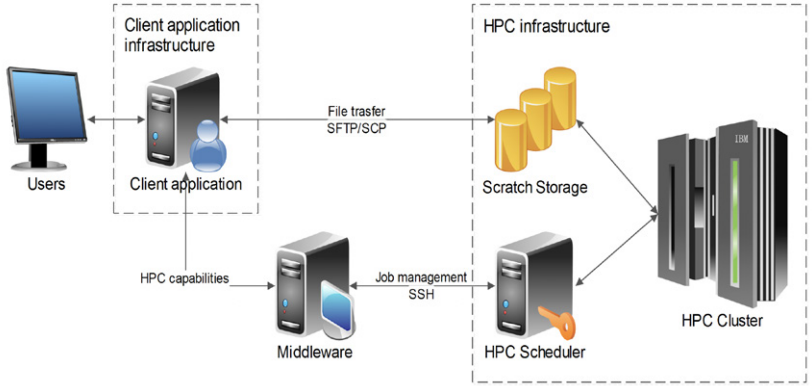
HPC platforms for scientific workflow execution

In the last issue of our Newsletter, we presented you with the first of the IT4Innovations research and development flagships — ESPRESO — Highly Parallel Finite Element Package for Engineering Simulations. In this issue, we would like to present the project called HPC platforms for scientific workflow execution, which is the second research flagship of IT4Innovations National Supercomputing Center.

Most supercomputing centres have set themselves the goal of lowering entry barriers to the world of high--performance computing for all users from research institutions, industry, state administration, hospitals, and other institutions without sacrificing execution performance. To this end, IT4Innovations' research activity in the areas of distributed systems, scheduling, remote execution, and security has been intensified.

The flagship research team is focused on the development of the HPC-as--a-Service concept (HaaS), which is a complex solution for HPC centres to make their HPC services available to a much broader user base. HPC-as--a-Service allows users to access HPC infrastructure without having to buy and manage their own physical servers or data centre infrastructure. Moreover, this approach lowers the entry barrier for everybody who is interested in using massively parallel computers, but often lacking the necessary level of expertise in this area. IT4Innovations has long been developing these HPC platforms and related software packages (HyperLoom, HEAppE, etc.), which are not dependent on just one type of infrastructure and as such they can be run by other supercomputing centres allowing them that can offer these packages to their users. Through the development of platforms, the user base is broadened to include academia, SMEs, and industrial companies that can take advantage of the HPC technology without an upfront investment in the hardware.

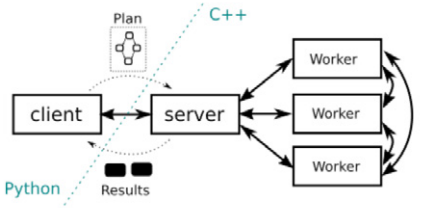
Simultaneously, a large portion of HPC workloads are scientific pipelines composed by domain specialists who do not have deeper knowledge and experience of and with HPC technologies, respectively. Therefore, the objective of the flagship research team is also to continue in the development of programming models allowing users to easily define dependencies between various computational tasks as well as runtime layers capable of their efficient execution in large scale distributed environments (e.g., HyperLoom software). Last but not least, the objective is also to make results available thus maximizing their potential impact.



HYPERLOOM

HyperLoom is a set of tools for defining and executing workflow pipelines in large-scale distributed environments. Not only it provides Python API to describe workload and its dependencies in abstract way but also it allows efficient runtime to execute pipelines containing millions of tasks on hundreds to thousands of nodes.

The HyperLoom tools have been developed independently of the used infrastructure. They can be operated on both an HPC cluster and cloud infrastructure.



http://www.hyperloom.eu

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HEAPPE (HIGH-END APPLICATION EXECUTION MIDDLEWARE)

To provide simple and intuitive access to a supercomputing infrastructure, an application framework called HEAppE has been developed. This framework utilizes a mid-layer principle, which is known as middleware in software terminology. Middleware manages and provides information about submitted and running jobs and their data transferred between a client application and an HPC infrastructure. HEAppE has been developed within a joint project of IT4Innovations National Supercomputing Center and the transnational DHI company, which is one of the leaders in the field of hydrological software development.

Primarily developed for application at IT4Innovations in the field of hydrological modelling, HEAppE has already been both used in many different fields and operated by several supercomputing centres.

The HEAppE platform is intended not only for one particular type of hardware for the existing high-performance and future exascale computing systems but also for the use of different systems in different supercomputing centres. By means of HEAppE, all interested parties may benefit from HPC technologies. HEAppE allows execution of required computations and simulations on HPC infrastructure, monitor the progress, and notify the user should the need arise. It provides necessary functions for job management, monitoring and reporting, user authentication and authorization, file transfer, encryption, and various notification mechanisms.

http://heappe.eu

AI – MLOC & HEAPPE

MLoC stands for an open-sourcee Machine Learning as a Service solution developed in order to lower the entry barrier to large-scale machine learning. It allows users to define artificial neural network architectures and manage their states through the REST API. MLoC features multiple supporting layers where Neural Network lifecycle numerical operations may be executed depending on their computational complexity.

Computationally demanding tasks, with low latency constraints, such as a neural network training may be offloaded to IT4Innovations HPC infrastructure. In contrast, lightweight tasks, such as model inference, expecting a quick response rate may be executed directly on the API infrastructure. MLoC closely operates with Heappe - IT4Innovations internal application framework.

https://github.com/it4innovations/mloc

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USE CASES

A very important part of this flagship activity is to ensure the impact on the end user. The above-mentioned technologies have already been used before and are currently used in a number of projects.

INVESTIGATORS

- Dr Jan Martinovic
- Dr Stanislav Böhm

NATIONAL PROJECTS

- Floreon+ – The evaluation of information to support decision-making within crisis management processes, namely floods. The development of a system to monitor, model, predict and support solutions to crisis situations, with a special focus on the Moravian - Silesian Region.
  www.floreon.eu
- MOLDIMED – The main objective of the platform is to provide researchers focused on clinical massively parallel sequencing data with easy and intuitive access to the HPC infrastructure via a specialized web interface.

www.floreon.eu

INTERNATIONAL PROJECTS

- ESA – the European Space Agency launched an initiative entitled Thematic Exploitation Platform (TEP), the objective of which was to develop and implement a set of thematically oriented platforms, virtual environments facilitating Earth observation generated data search.
- ExCAPE – Within the project, IT4I was involved in development of state-of-the-art scalable algorithms and implementations suitable for running on future exascale machines.
- LEXIS – The objective of the project is to build an advanced engineering platform leveraging modern technologies from High Performance Computing, Big Data, and Cloud Computing.
  lexis-project.eu
- ExaQUte – The aim of the three-year long project ExaQUte is to develop new methods for solving complex engineering problems using numerical simulations on future exascale systems.
  www.exaqute.eu

lexis-project.eu **www.exaqute.eu**

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PUTTING AN END TO THE USE OF CHEMICAL CROP SPRAYING USING WEED DETECTION

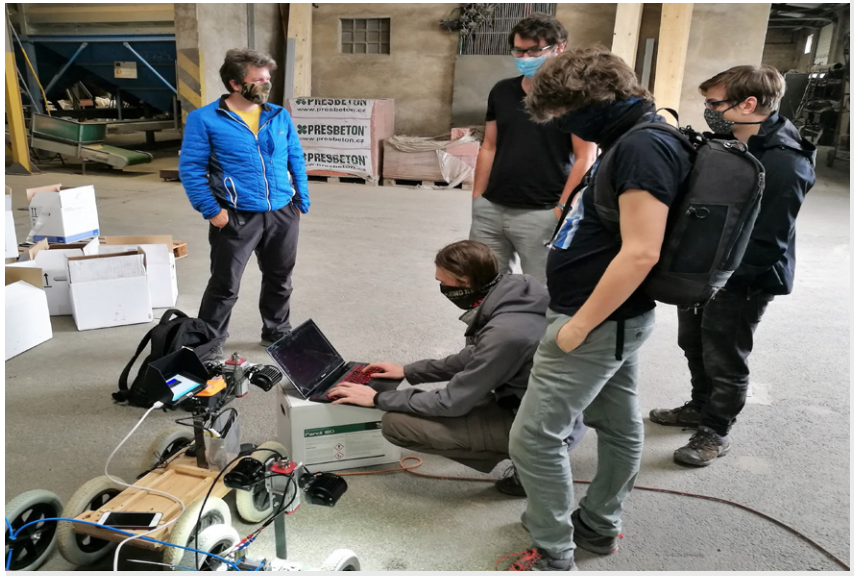
Putting an end to the use of chemical crop spraying using weed detection

In early 2020, the Digital Innovation Hub Ostrava (DIH Ostrava) was established, bringing together the activities of IT4Innovations and MSIC Ostrava, enabling small and medium-sized enterprises to examine and potentially address their digitalisation needs. These, unlike large companies, tend not to have the financial or human resources to commit to verifying and potentially deploying digital technologies. For this reason, the Moravian-Silesian Region also decided to support the foundation of DIH Ostrava, including a pilot financial advantage tool for selected types of services and access to supercomputing capacities.

One of the supported projects is also that of Ullmanna, a company developing an agricultural weeding machine that would allow line weed control by recognizing the target crop through machine learning. This would lead to performing agricultural activity without the use of chemical sprays.

"Our intended product has a significant positive impact on both the environment and society, allowing an increase in food production without the use of pesticides, which negatively affect both the environment and human health," says Martin Ullmann from the Ullmanna company.

This project uses machine learning to automatically recognize crops from weeds. Within IT4Innovations, a neural network is being designed and trained to do this. Crop recognition mechanism will allow the weeding machine to remove weeds and not to damage the cultivated crop. Due to the direct deployment on the weeding machine, additional requirements are placed on the resulting technology regarding the HW used and the recognition speed.



Moravian-Silesian Region

The subsidy for the "Digital Innovation Center Ostrava – Pilot Verification" project is provided from the budget of the Moravian-Silesian Region (Contract No. 08183/2019/RRC)

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EVENTS TAKEN PLACE IN AND WITH OUR CENTRE

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IT4INNOVATIONS HONOURED BY THE VISIT OF THE FRENCH EMBASSY ATTACHÉ

At the beginning of October, we welcomed at IT4Innovations the Scientific and Higher Education Attaché for the Embassy of France in the Czech Republic, Mrs. Veronique Debord-Lazaro. The subject of the meeting was a discussion on cooperation in research and development with French institutes and on the possibility of educating Czech students under the cotutelle regime, which was brilliantly outlined in the presentation by Tomáš Kozubek, the IT4I Scientific Director. As part of her visit, Mrs. Veronique Debord-Lazaro inspected the IT4Innovations infrastructure and got a closer look at the work of the Modelling for Nanotechnologies Lab.

VISIT OF THE AMBASSADOR AT IT4INNOVATIONS

In mid-September, we had the honour to welcome Jaroslav Zajicek, who holds the post of Deputy Permanent Representative of the Czech Republic to the EU. The ambassador was accompanied by his deputy Lucie Sestakova, Vice-President of the Union of Industry and Transport of the Czech Republic Jan Rafaj and others, who had the opportunity to discuss with the management of IT4Innovations the activities of our supercomputing centre the possibility of cooperation with industrial enterprises.

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TRAININGS AND EXCURSIONS IN THE COVID ERA

Despite the difficult situation, we managed to organize the Parallel Visualization of Scientific Data using Blender course, organized by IT4Innovations and PRACE and led by Petr Strakos, Milan Jaros, and Alena Jesko on 24th September.

Currently, with emergency measures not allowing excursions and trainings, a lecture can be organised for schools or other institutions online. One such virtual lecture by Tomas Kozubek, the Scientific Director, took place on 30th September for students at Grammar School and the Business Academy Orlova.

WE HOSTED A ROADSHOW OF THE CZECH RADIOCOMMUNICATIONS

On 24th August, the representatives of the municipalities of the Moravian-Silesian Region met at IT4Innovations, where we hosted a roadshow of the Czech Radiocommunications. It has brought interesting information to all participants about the transition to the new terrestrial television broadcasting standard. The mayors and representatives of the municipalities were informed of the steps needed to maintain the free terrestrial reception of the broadcaster and had the opportunity not only to address their questions on this subject but also to tour the IT4Innovations infrastructure.

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