NEWSLETTER Q1/2019

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

INVITATIONS

HIGH PERFORMANCE COMPUTING IN SCIENCE AND ENGINEERING (HPCSE) CONFERENCE

20th–23rd MAY 2019, HORSKÝ HOTEL SOLÁŇ, BESKYDY MOUNTAINS

The HPCSE conference is held every two years, and this year the conference will have already been organized for the fourth time. Its primary objective is to present the latest research results in applied mathematics, numerical linear algebra, optimization methods, computational sciences, and HPC. This year, it is taking place on 20th to 23rd May 2019.

hpcse.it4i.cz/HPCSE19

DATA SCIENCE WITH R AND PYTHON COURSE

24th–25th APRIL 2019, IT4INNOVATIONS

The two-day Data Science with R and Python course will take place at the end of April and will be led by our colleagues Tomáš Martinovič and Stanislav Böhm. The first and the second day of the course will be dedicated to the R and Python programming language, respectively.

training.it4i.cz/DataSci-04-2019

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IN BRIEF

THE EUROPEAN COMMISSION BLOG DEDICATED TO THE DIGITAL SINGLE MARKET

Our centre has been registered by the European Commission as a Digital Innovation Hub for cooperation with industry in the field of HPC and advanced data analysis. Apart from the detailed information included in the EC online catalogue, you can also find IT4Innovations in the article “IT4Innovations: HPC at the Heart of a Digital Innovation Hub” by Tomáš Karásek on the EC blog.

ec.europa.eu/digital-single-market/en/blogposts/it4innovations-hpc-heart-digital-innovation-hub

NEXT OPEN ACCESS GRANT COMPETITION WILL BE LAUNCHED IN JUNE 2019

In June 2019, the 17th Open Access Grant Competition will be launched for you to apply for the IT4Innovations computational resources. Please, visit our website for updates.

www.it4i.cz

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NVIDIA DGX-2

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Artificial intelligence research gets green – we have expanded our infrastructure with NVIDIA technology

Our brand-new NVIDIA DGX-2 computing system was officially launched on 4th March 2019, and as such it is the first ever installation of this type in Central and Eastern Europe. The system is designed to tackle the most challenging artificial intelligence tasks, delivering over 2 PFlop/s of performance for AI researchers. The ceremony was attended by Ivo Vondrák, the Governor of the Moravian-Silesian Region, Tomáš Macura, the Mayor of the City of Ostrava, and Václav Snášel, the Rector of VSB – Technical University of Ostrava.

NVIDIA DGX-2 supplied by M Computers, a Czech-based company, will be made available to a broad base of users from academic, research, and commercial institutions from the Czech Republic and abroad.

"Our main mission is to enable Czech scientists to access high-tech technologies. This new GPU-accelerated system will allow them to keep up with the world in the field of artificial intelligence, which, together with digitisation, we consider to be the key to the development of society. That's why we decided to buy this unique system" said Vít Vondrák, managing director of IT4I.

NVIDIA DGX-2 is equipped with 16 of the most powerful data centre accelerators – NVIDIA V100 Tensor Core GPUs. They are inter-connected with revolutionary NVSwitch technology that delivers a total bandwidth of 2.4 TB/s. In official documents, reference is made to 2.4 TB/s. However, Jensen Huang, the NVIDIA CEO, in his presentation speaks of some 14.4 TB/s, comparing it to HD movie transmission. To illustrate this, DGX-2 would be capable of transmitting 1,440 HD movies (10 GB each) per second.

The systems include 512 GB of HBM2 memory. NVIDIA DGX-2 also offers 30 TB of internal capacity on fast NVMe SSDs. Inter-connection to the surrounding infrastructure is provided via eight 100 Gb/s Infiniband/Ethernet adapters.

One NVIDIA DGX-2 can replace 300 dual--socket servers with Intel Xeon Gold processors for deep neural network training (ResNet-50). DGX-2 is powered by the DGX software stack – NVIDIA-optimized and tuned AI software that runs the most popular machine learning and deep learning frameworks with maximized performance. NVIDIA DGX-2 can also be used for traditional HPC workloads to deliver a theoretical peak performance of 130 TFlop/s.

The extension of the IT4Innovations infrastructure is supported by the European Regional Development Fund under the project IT4Innovations National Supercomputing Center – Path to Exascale, CZ.02.1.01 / 0.0 / 0.0 / 16_013 / 0001791, implemented from the Operational Program Research, Development and Education of the Ministry of Education, Youth and Sports of the Czech Republic.

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

MINISTRY OF EDUCATION, YOUTH AND SPORTS

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NVIDIA DGX-2 launching ceremony, 4th March 2019

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Large-scale EXecution for Industry & Society

LEXIS

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We have successfully launched the first Horizon 2020 project coordinated by VSB-TUO: LEXIS

Between 14th and 16th January 2019, the LEXIS (Large-scale Execution for Industry & Society) project funded from the EU's Horizon 2020 framework programme was kicked off at VSB – Technical University of Ostrava with our colleague Dr Jan Martinovič being its Principal Investigator. It is the first H2020 project coordinated by VSB – Technical University of Ostrava.

The kick-off meeting of the LEXIS project partners' consortium, officially launching the project implementation, was held in Ostrava in January 2019. 16 partners from all over Europe gathered here and joined forces to set up all activities to be completed during the project. LEXIS brings together a consortium with the skills and experience to deliver a complex multi-faceted project, spanning a range of complex technologies across seven European countries.

Project coordinator Dr Jan Martinovič clearly defines the immediate ambition of LEXIS: "Our target is to build an advanced engineering platform leveraging modern technologies from High Performance Computing (HPC), Big Data, and Cloud Computing. We will demonstrate the benefits of the LEXIS project in the context of three industrial large-scale pilots which are Aeronautics, Weather & Climate, and Earthquake & Tsunami."

Combinations of HPC, Cloud and Big Data technologies are key to meeting the increasingly diverse needs of large and small organizations alike. Critically, access to powerful compute platforms for Small to Medium Enterprises - which has been difficult due to both technical and financial reasons - may now be possible.

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ISO 27001 INFORMATION SECURITY CERTIFICATE

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WE HAVE BEEN AWARDED THE ISO 27001 INFORMATION SECURITY CERTIFICATE

Since December 2018, IT4Innovations National Supercomputing Center has been an Information Security Management System certificate holder according to the international ISO/IEC 27001:2013 (Czech version: ČSN ISO/IEC 27001:2014) standard.

The ISO 27001 certificate has been awarded for the following areas:

- provision of national supercomputing infrastructure services,
- high-performance computing problems solutions,
- performance of advanced data analysis and simulations, and
- processing of large data sets.

Certification according to this standard certifies that IT4Innovations plans, maintains, evaluates, and continually improves its information security management system. In the field of information security, it includes continual risk management, defining security policies, evaluating the efficiency of adopted measures, mitigating potential impacts, raising the security awareness of employees, managing interactions with economic operators, and securing other security aspects at the organisational and administrative, personal, physical, and cryptographic levels.

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TWELVE-DAY FIJI HACKATHON

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From Thursday 17 January 2019 through Tuesday 29 January 2019, IT4Innovations hosted a FIJI Hackathon focused on parallelization and HPC. Fiji (Fiji Is Just ImageJ) is a popular software platform for image processing, and its community has developed and made available numerous plugins for scientific audiences.

A Hackathon is an event where scientists with programming skills come together to solve problems. The FIJI Hackathon is a two-week brainstorming session where they work in a low-distraction, high-energy environment to advance the software side of their research. Typically, results are accomplished more easily during these hackathons because the setting is ideal to discuss advanced ideas with similar-thinking scientists and ideas can sprout much faster.

FIJI Hackathons have been organized regularly since 2007. Previous hackathons took place, for example, in the USA, Germany, Switzerland, and France. It was held in the Czech Republic for the first time, and attended by 28 developers altogether.

Pavel Tomančák

An interview with the organizer of the Fiji Hackathon in Ostrava

We asked Pavel Tomančák, who organized the hackathon at IT4Innovations:

You are the godfather of Fiji, can you share with us the origin of the software platform?

"I am a biologist and back in 2008 I wanted to use an advanced, so-called light sheet microscope, for imaging Drosophila embryos. We had the microscope, but in order to use the data they had to be processed in a computer. The algorithms to do that were either not readily available or even non--existent and therefore I had no choice but to develop them. I hired students with computer science background and they did it (both of them have their own labs now). Since I am not a card-carrying computer scientist, and programming is more a hobby for me, from the beginning I was asking myself: ‚What will happen when those students leave my group? Will the software they developed keep working?' The solution was to embed it into a larger platform that has a community of developers who would maintain the software in the long run. At the time, ImageJ was an obvious choice, since many biologists were using it, and it is open source. Coincidentally, at the time my good friend Albert Cardona was visiting my lab in Dresden. Albert used ImageJ for pretty much the same purpose in a different field of bioimaging (electron microscopy). Together with a mathematician, Johannes Schindelin, they were developing a new distribution of ImageJ that is able to install and run at the time a very complex program that Albert was developing. Since I was a PI, had money, and needed the platform to develop my own tools sustainably, I hired Johannes, and together with Albert we started to work on, promote, and support Fiji. We would never have guessed that the program would have about 75,000 users around the world ten years later. We were just solving our own problems.

As far as the name is concerned, Fiji is a self-referential acronym, something rather popular among geeks, I mean computer scientists. It stands for Fiji Is Just ImageJ and it highlights that fact that

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Fiji has its roots in ImageJ and extends it towards various challenging biology applications. In reality, Albert came up with the name because his girlfriend at the time liked Fiji. We just rationalized it later “

What was the main purpose of this year’s hackathon, and how can one participate at those events?

“Hackathons are usually very free-wheeling events. Everybody comes to work on his/her problem and benefits from having all this expertise in one room. Instead of going online and asking, you can just walk over to a developer of a particular part of Fiji on which your project depends and work together on solving any issues. Since we were holding the hackathon at IT4I, we had a general theme to work on Fiji’s ability to run on a supercomputer. There was a lot of progress in this direction. So far, it is all under the hood, but soon this kind of infrastructure will enable Fiji users world-wide to deploy really big computations on gigantic microscopy datasets on their own clusters or even remotely, using the excellent hardware at IT4I. Hackathons are for expert programmers, no one is going to really hold your hand on the basics, we usually invite only seasoned developers. But we also organize so-called Learnathons (so far mostly in Dresden) where we bring less advanced Fiji hackers up-to-speed with the latest software engineering infrastructure. And these people often later end-up coming to a Hackathon.“

Can you provide us with a brief summary of overall accomplishments of this year’s FIJI Hackathon?

“We had many new people this year who got to know each other, and that is always the major accomplishment of such an event. Of course, lots of code was produced and this process continues. We call it a ‚hackathon effect‘ – people come so energized from the intense two weeks of hacking that they soon finish many of the projects they started during the hackathon. One can easily visualize that by looking at the code repository on github. Hackathons are really remarkable events for the Fiji community, where many things move forward (for example the HPC integration).

This year, we discovered a great new hackathon venue. The hotel was right next to the IT4I building, the weather was frigid, air-pollution high, and so there was essentially nothing else to do than program most of the time. There was even a strategically positioned restaurant (Stračena) and pub (Kurnik Šopa) within walking distance. The perfect environment for a hackathon. We will come back to Ostrava.“

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This year two open lectures on "Content-Aware Image Restoration for Light and Electron Microscopy" and "KNIME Image Processing: Status Quo and Future Directions" by invited foreign experts, Florian Jug and Christian Dietz, were included. And for those who could not attend the open lectures, we asked Florian Jug:

You talked about content-aware image restoration (CARE) techniques, can you briefly explain this research of yours?

"Modern microscopes can record many hours of 3D time-lapse movies of every cell in entire developing organisms. Just like in regular photography, fluorescence microscopy requires a sufficient amount of light to avoid dark and noisy images. However, the amount of light needed for such movies can easily reach levels that harm frequently studied model organisms such as worms, fish, or mice. So far, the only option to avoid this "ultimate sunburn" is to record shorter movies or reduce the amount of light. As a consequence, many biologists are forced to work with very noisy images that are hard to interpret.
Together with my colleagues at the Center for Systems Biology Dresden (CSBD) and the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), we have now developed a content-aware image restoration method – CARE – that solves this dilemma. CARE is based on artificial neural networks and reveals the content hidden in low-quality microscopy images. With these new methods biologists are now able to restore high-quality microscopy images, even if acquired with up to 60 times less laser light, enabling imaging experiments that had not been possible before. This new method is fully open-source and can be found on GitHub. We designed it to be easy to use and can, if required, be adapted by anyone."

Are you willing to share with us the most impressive memories from your stay at IT4Innovations in Ostrava during the hackathon?

"Honestly, we all had an absolutely great time here at IT4Innovations. Since leading a research group requires a lot of time, I usually have only very limited time to sit down and code. Here in Ostrava I was almost a post-doc again, it was such a treat! Despite this, I will certainly not forget the tour through your impressive cluster facility and our visit to the coal mine you organized. It is not the first time I saw a cluster, but I was truly impressed.

Last but not least I have to mention the food and the beer... OMG! Of course everybody knows how good Czech beer is, but the beer we got served here was better than any Czech beer I can buy in Germany. Once back home I think I will have to go running a bit more frequently in order to lose some extra weight I might have gained in Ostrava... ;)"

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We also asked Christian Dietz:

You spoke about KNIME image processing, can you give a brief introduction to this open-source platform?

"The KNIME Analytics Platform is an easy to use and comprehensive open source data integration, analysis, and exploration platform designed to handle large amounts of heterogeneous data. The over 2,000 available modules ("nodes") cover each step of a data analysis workflow; they integrate data types and functionality from various domains, including image processing, cheminformatics, and bioinformatics. Many of these nodes are provided through open source integrations, e.g. Keras and Tensorflow for deep learning, Apache Spark for big data processing, H2O for high performance machine learning, Python and R for scripting and plotting, RDKit for cheminformatics, to name only a few.

The KNIME Image Processing extensions for the KNIME Analytics Platform integrate well-known open source tools from the field of bioimage analysis (e.g. ImageJ2/FIJI, ImgLib2, OMERO, Ilastik, BigDataViewer and CellProfiler). Leveraging the functionality that is provided by the KNIME Analytics Platform, users can design complex end-to-end image analysis workflows, capable of processing multi dimensional images and videos at a large scale through to the subsequent machine learning, statistical analysis, or visualization."

You have attended FIJI Hackathons quite regularly since 2011, can you tell us what you like most about taking part in them, and what caught your attention the most about the one at IT4Innovations?

"From my point of view, hackathons are great for two reasons: first, you get to work with people you usually work with only remotely. Over time, you make friends in the community and at the hackathons you have the chance to hang out with them. Face-to-face meetings often provide the better ground for developing new ideas and motivation. Second, you can focus on a specific project for a certain amount of time without any distraction from your daily work (if you plan it the right way).

At the IT4Innovations Hackathon, the two aforementioned points were fully met. But also getting the opportunity to meet new people, new to the field of bioimaging, but with a strong expertise in HPC, was a great experience from which I learned a lot. I'm eager to keep my new contacts and am looking forward to future collaborations."

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This event was supported by the ERDF in the IT4Innovations national supercomputing center - Path to Exascale project (CZ.02.1.01/0.0/0.0/16_013/0001791) within the OPRDE.

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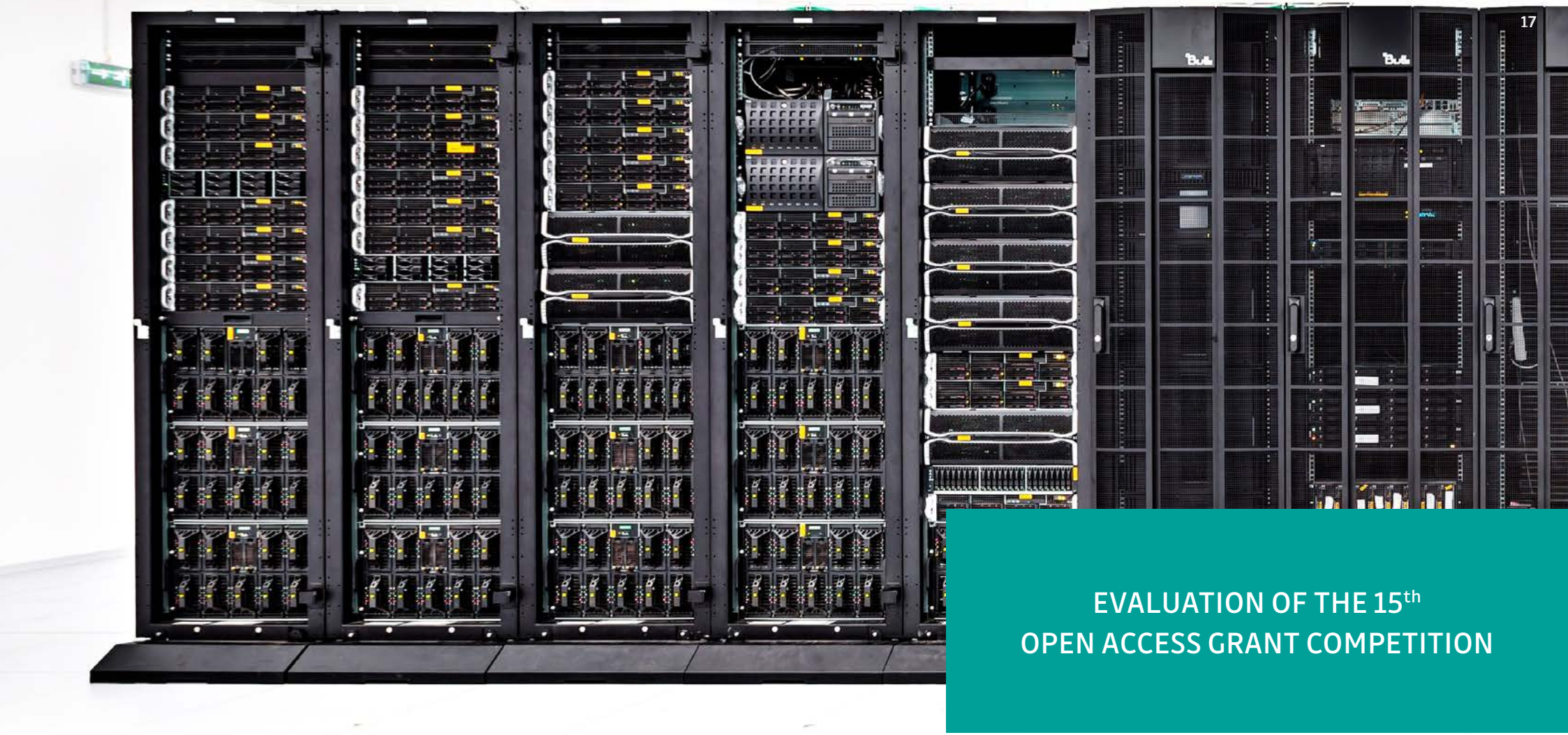

EVALUATION OF THE 15th OPEN ACCESS GRANT COMPETITION

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Within the 15th Open Access Grant Competition, applicants applied for almost 105 millions of core hours. The requested resources thus exceeded the reserved capacity by 119 %. Therefore, the allocation committee again had to decrease the computational resources to be allocated to most of the evaluated projects, and distributed a total of 69.3 millions of core hours among 71 successful projects.

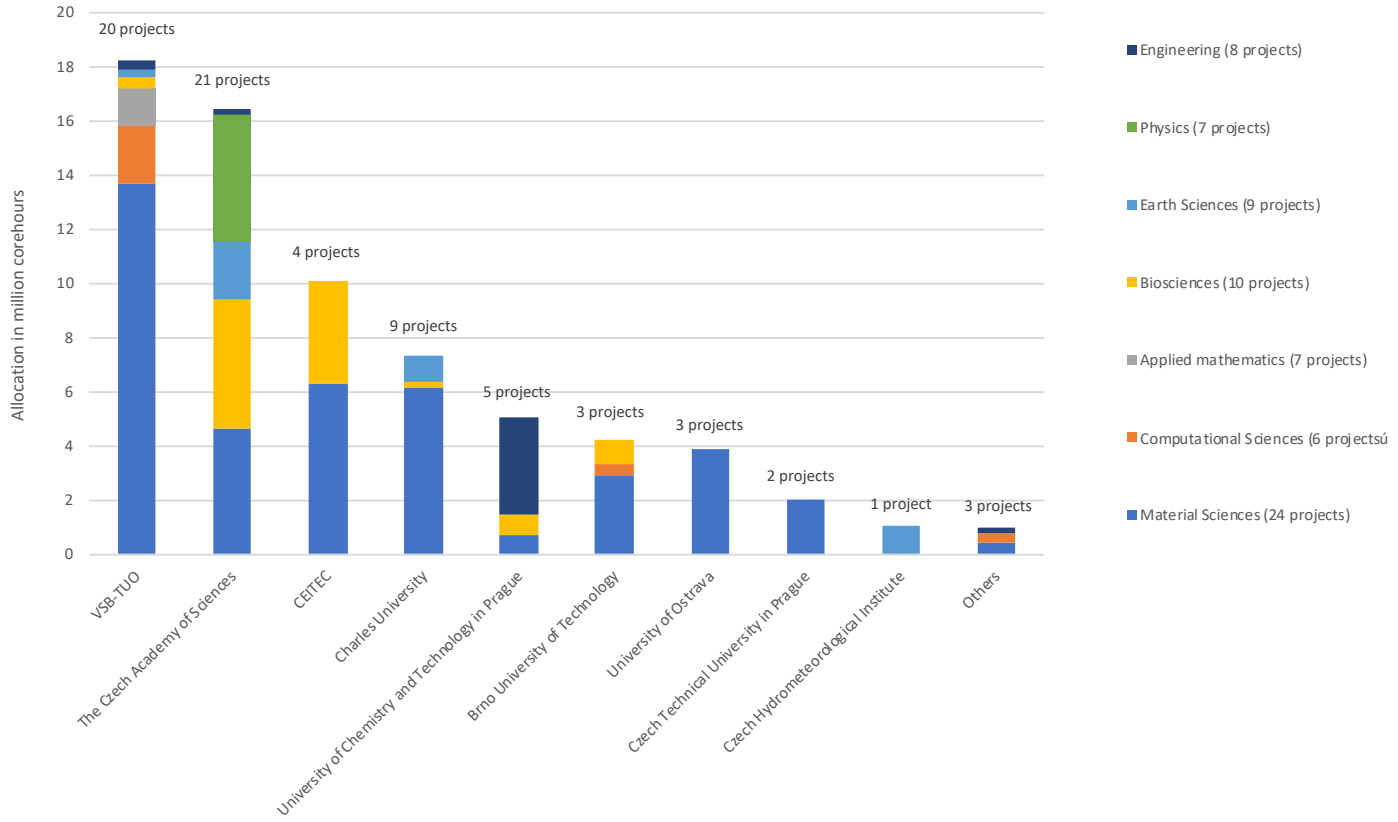
In total, 91 % of computational resources were allocated to 41 projects, which passed the technical evaluation as well as the evaluation of the allocation committee. The most frequent scientific domains included material sciences, followed by biosciences and Earth sciences. A total of twenty projects were granted more than 1 million core hours each. The Principal Investigators of these "million" projects are researchers from 9 different research institutes such as IT4Innovations, CEITEC, the Czech Academy of Sciences, Charles University, the University of Ostrava, the University of Chemistry and Technology in Prague, Brno Technical University, the Czech Technical University in Prague, and the Czech Hydrometeorological Institute.

The projects of applicants who applied for 400 thousand core hours or less had to pass the technical evaluation only, and the required resources were allocated to them in full. These 30 projects were granted a total of 9 % of the total number of allocated core hours. Like in the 14th Open Access Grant Competition, the majority of the projects fall in engineering research (7) and applied mathematics (6).

As far as organizations are concerned, a quarter of the total reallocated computational resources was awarded to the projects of VSB-TUO (primarily IT4Innovations) applicants. Another quarter of these resources was awarded to 7 Czech Academy of Sciences institutes, the projects of which are amongst most successful. A total of 21 projects of this public research institute were awarded almost 16.5 million core hours.

Apart from the projects of the universities and research institutions presented in the graph below, projects of Tomáš Baťa University in Zlín, the University of Pardubice, and the University of West Bohemia in Pilsen were also awarded computational resources.

Allocation of computational resources in the 15th Open Access Grant Competition by research domains and organizations



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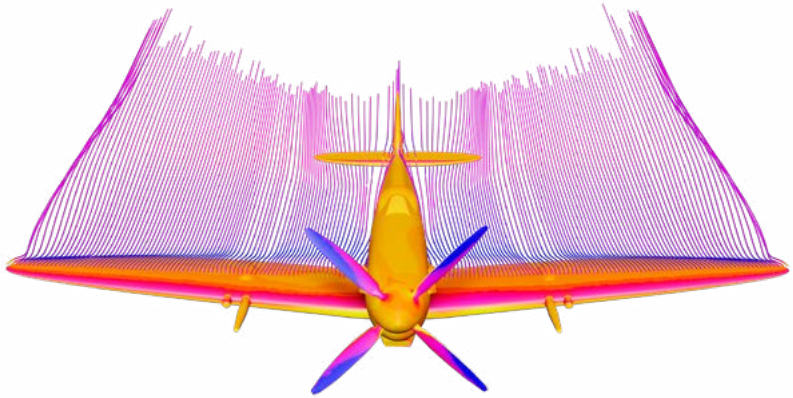
Synthetic fingerprint of an eczema-affected finger –
note the long white lines running oughout the whole fingerprint



Output of the prepared and already mentioned tool
for visualization of scientific data using Blender

Jan Tinka
Brno University of Technology

MACHINE LEARNING IN BIOMETRICS AND BIOMEDICINE

The computational resources amounting to almost 1 million core hours will be used by scientists from Brno University of Technology for development of automated detection system for diabetic retinopathy, and for removing the effects of skin diseases for fingerprint recognition. Retinopathy often refers to a retinal vascular disease, or damage to the retina caused by abnormal blood sugar. A higher risk of development of various forms of this disease is present in diabetes patients.

The objective of the project of Jan Tinka and his team is to develop a detection system using machine learning algorithms, the use of which will be user-friendly for eye specialists as well as patients. In cooperation with dermatologists, Jan Tinka is also developing a system for detection, localization, and recognition of fingerprint damage.

Dr Petr Strakoš and Dr Lubomír Říha
IT4Innovations

RESEARCH AND DEVELOPMENT OF LIBRARIES AND TOOLS IN THE INFRA LAB

Our colleagues from the IT4Innovations Infrastructure Research Lab were awarded almost 1.5 million core hours for developing the tools used by the users of our supercomputers in their research. The key topics of this project include energy efficiency in HPC, development of the numerical ESPRESO library, and visualization tools.

The allocated computational resources will be used for analysis of the behaviour of new HPC applications and their dynamic tuning, with the objective to reduce the energy consumption when run on a supercomputer. In the case of the ESPRESO library, one of our research flagships, the research will be focused on solutions for, for example, improving single-node performance and in its deployment on systems with graphic accelerators. As far as the visualization tools are concerned, our colleagues aim to develop an open source tool for the visualization of scientific data which will be available to the users of our infrastructure. The visualization tool will be based on Blender, the popular 3D creation suite, in particular on its 2.80 version, which is to be released in the first quarter of this year.

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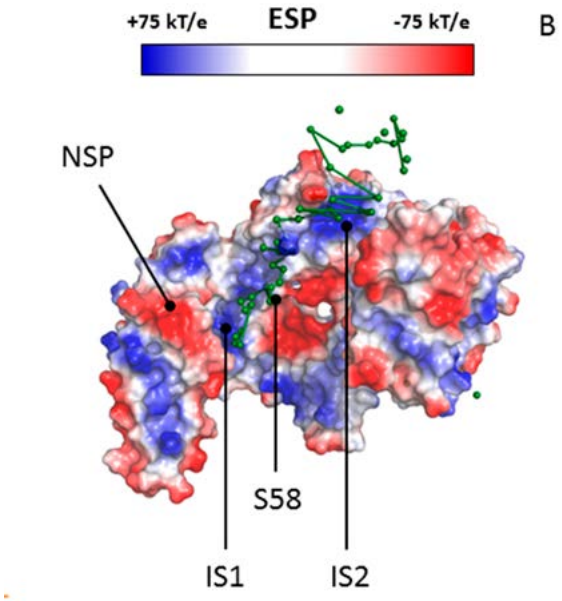

Conserved association pathway of phosphorylated partners to the primary binding location (IS1) of the 14-3-3 protein is shown in green. The image is taken from the publication NAGY, G., C. OOSTENBRINK, J. HRITZ a Y. Koby LEVY: Exploring the Binding Pathways of the 14-3-3ζ protein: Structural and Free-energy Profiles Revealed by Hamiltonian Replica Exchange Molecular Dynamics with Distancefield Distance Restraints. PLOS ONE. 2017, 12(7). DOI: 10.1371/journal.pone.0180633.

Dr Jozef Hritz
Masaryk University

COMPUTATIONAL CHARACTERIZATION OF SELECTED PROTEINS ASSOCIATION FREE ENERGIES II

Already the seventh project of Dr Hritz from Masaryk University was awarded computational resources of IT4Innovations. He uses supercomputers, for example, for his research of the 14-3-3 protein complexes and tyrosine hydroxylase (TH).

His project submitted within the 15th Open Access Grant Competition was awarded more than 1.5 million core hours. The research objective is to reveal structural and free energy changes, which are essential for protein complexes' formation. Any disruption of the network of interactions underlying the formation of protein–protein complexes may lead to a number of pathologies.

His research group will also focus on TH, one of the key enzymes operative in the human brain. The TH/14-3-3 protein complex regulates the level of dopamine, an organic chemical which plays an important role as a neurotransmitter, and of which deficiencies are heavily implicated in the onset of Parkinson's disease. By combining state-of-the-art computer simulation and contemporary experimental techniques (e.g., nuclear magnetic resonance and cryoelectron microscopy), better understanding of the dynamical properties and thermodynamics of protein association will be possible.

Using strengthened sampling computational methods, Dr Hritz's research team has, for example, already discovered that the 14-3-3 protein must adopt a transitional conformation state not known up till now. Moreover, they discovered a conserved associated pathway serving client proteins to reach their final binding conformation once they are phosphorylated. These findings can be useful in explaining the effects of mutation along this association pathway as well as in its use as the target for designed drugs modulating this group of the 14-3-3 protein complexes.

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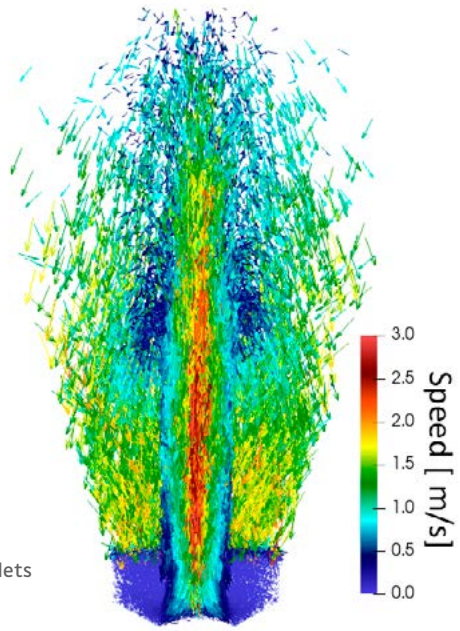

Illustration of the typical movement of pellets in the Wurster fluid bed coater

Jiří Kolář
University of Chemistry and Technology

INVESTIGATION OF FLUIDIZATION REGIMES IN WURSTER FLUID BED COATER

The Wurster fluid bed device is widely used in pharmacy for the coating of small pellets. Coating is used to apply layers onto the pellets with various functions. Some layers can consist of active pharmaceutical ingredients (API), and others can be used to protect the API from decomposing, or prolong the drug effect. However, it is difficult to set the process operating parameters optimally to obtain product of a pharmaceutical quality.

Being awarded almost 3 million core hours, the project of Jiří Kolář from the University of Chemistry and Technology in Prague is focused on analysis of dependency of fluidization regimes on operating parameters setting in a Wurster fluid bed coater using computationally intensive simulations. Jiří Kolář will then seek to find an optimal simplification of this model, which could have the capacity to speed up the drug design and reduce its costs.

Prof. Miroslav Vozňák
IT4Innovations the Faculty of Electrical Engineering and Computer Science at VSB-TUO

ANALYSIS OF CAUSES AND PREDICTION OF PCRF EVENTS IN 4G AND 5G NETWORKS

Our colleague Prof. Miroslav Vozňák and his team from the Faculty of Electrical Engineering and Computer Science at VSB-TUO were awarded almost half a million core hours for their project aimed at increasing the reliability and reducing the costs of maintaining new technologies to ensure mobile 4G and 5G network operation. This research is being carried out based on cooperation with the Centre of Excellence for network development operated by T-Mobile Czech Republic a.s. Together, they would like to find the key data sources, gather information about technical problems in one place, and identify performance indicators which can be used to increase reliability and prevent problems in the network.

The data processing results obtained by the use of a supercomputer will serve as the basis for planned machine learning applications such as detection and classification of mobile network anomalies.

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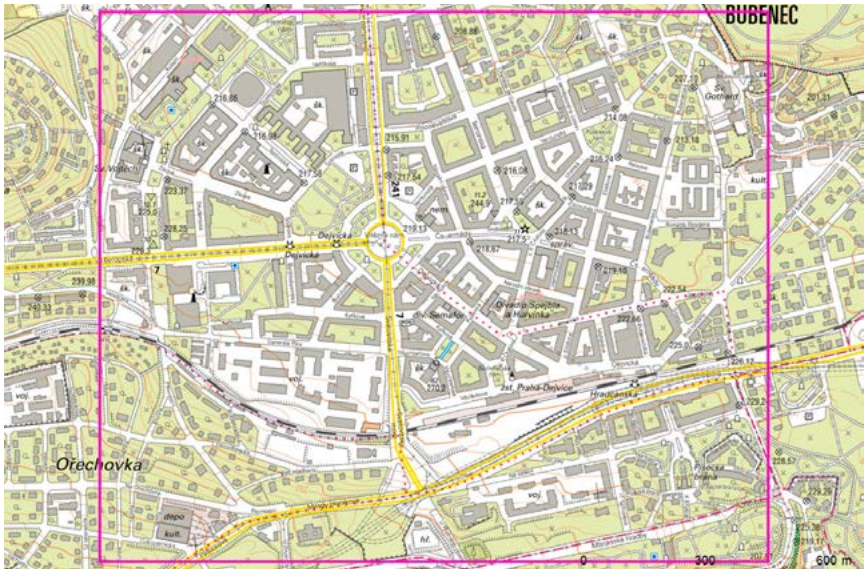

Computational domain of the PALM-4U model
in Praha-Dejvice area

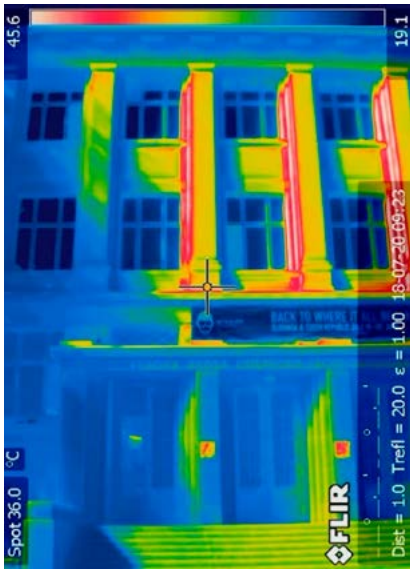

Image of a building in visible
and infrared spectra

Ondřej Vlček
the Czech Hydrometeorological Institute

VALIDATION OF THE MODEL PALM-4U AGAINST OBSERVATION CAMPAIGN IN PRAGUE-DEJVICE

PALM-4U (www.palm4u.org) is a micro-scale model which allows detailed simulation of meteorological conditions and air quality in urban areas with a resolution of single meters. Its use makes modelling of increasingly frequent extremely high temperatures in urban areas (Urban Heat Island Effect) followed by increased air pollution easier. Besides, the model also allows complex evaluation of urban scenarios' impacts on microclimate and air quality.

The project of Ondřej Vlček from the Czech Hydrometeorological Institute (CHMI) and his colleagues from Charles University and the Czech Academy of Sciences aims at carrying out detailed validation of the latest PALM-4U model against the observation campaigns done in the Praha-Dejvice area. The campaign measurements were conducted by CHMI specialists in two fourteen-day episodes with one taking place in the summer and the other one in the winter of 2018. They measured not only the meteorological conditions and air quality in street canyons, but also building surface temperatures and heat flow through facades using infrared cameras. The team will also have access to the data generated by Prague's meteorological stations.

For validation of the model, they closely collaborate with partners from the German MOSAIK project (Urban planning based on the model and its use in the climate change domain), and they were awarded more than 1 million core hours for this work within our 15th Open Access Grant Competition.

This work has been funded by the Operational Programme Prague – Growth Pole "Urbanization of weather forecast, air quality prediction, and climate scenarios for Prague" (CZ.07.1.02/0.0/0.0/16_040/0000383).

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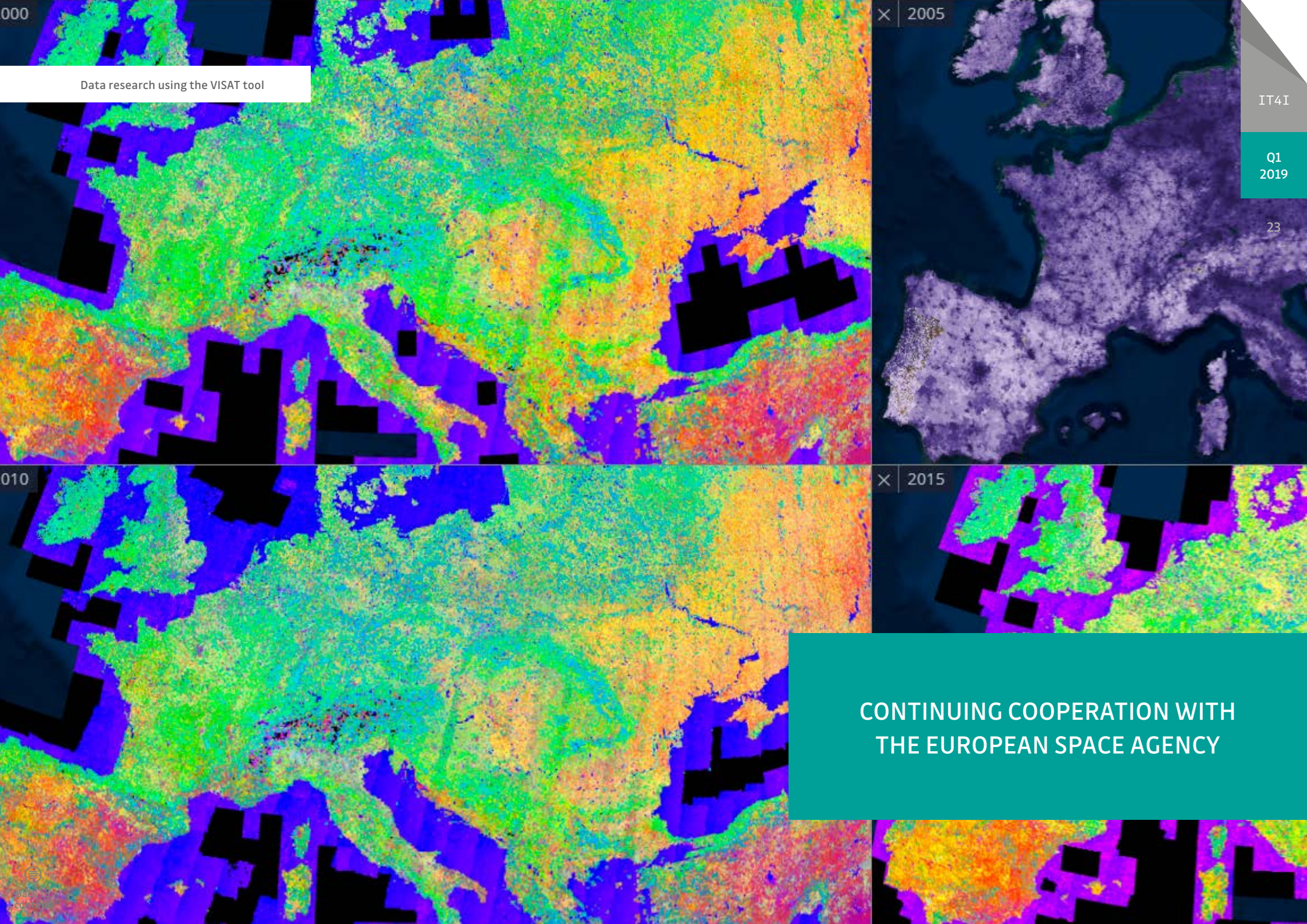
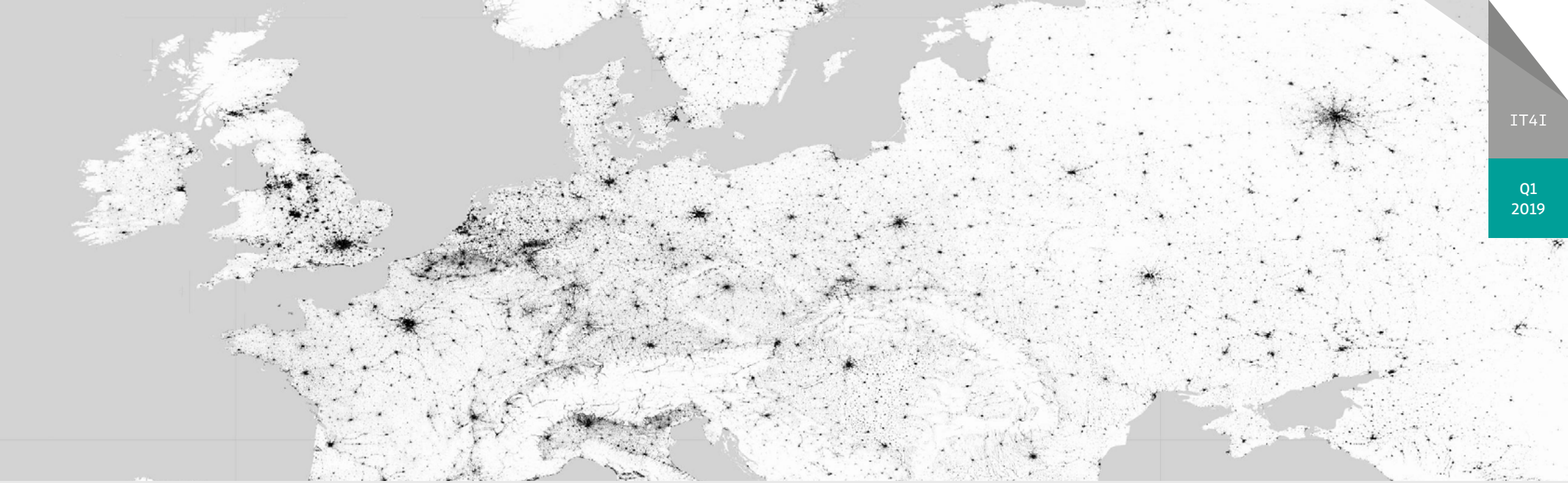


Data research using the VISAT tool

CONTINUING COOPERATION WITH THE EUROPEAN SPACE AGENCY



In 2014 the European Space Agency (ESA) started the initiative “EO Exploitation Platforms (EPs)” which represents a set of research and development activities aiming at the creation of an ecosystem of interconnected “Thematic Exploitation Platforms (TEPs)”. Basically, TEP is a collaborative, virtual work environment with one coherent user interface that provides access to EO data and the tools, processors, and data processing and storage resources required to efficiently extract thematic geo-information from mass EO data sources.

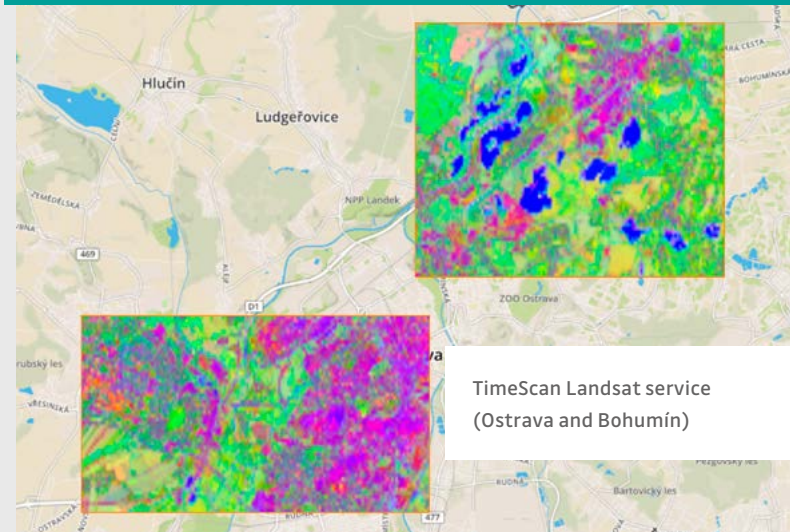
The Urban TEP platform is operated by an international consortium of five partners, including the German Aerospace Center (DLR, Germany), Brockmann Consult GmbH (BC, Germany), Terradue Srl (T2, Italy), IT4Innovations National Supercomputing Center (IT4I, Czech Republic) and Gisat s.r.o. (GS, Czech Republic).

The Urban Thematic Exploitation Platform (Urban TEP) aims at the utilization of modern information technology functionalities and services to bridge the gap between the technology-driven Earth Observation (EO) sector and the information needs of environmental science, planning, and policy. Key components of the system are an open, web based portal connected to distributed high-level computing infrastructures and providing key functionalities for data access, processing, analysis, and visualization, along with the possibility of customized development and sharing of algorithms, products and services via dedicated networking and communication tools. The Urban TEP platform offers a change in the use of EO data and geospatial analytics by enabling any interested user to easily exploit and generate thematic information on-demand.

By the end of 2018, the Urban TEP project entered its next phase with a focus on systematic enhancement and streamlining of the platform capabilities and functionalities. For the Urban TEP to become the fully operational and sustainable platform the project aims at development of tailored use cases for a group of current so-called early adopters and hopefully future customers of the platform.

These use cases include for example “UAV (Unmanned Aerial Vehicle) mapping service” for the World Bank Group, “Population exposure to hazards in SE-Asia” for the United Nations, “Slum area mapping” for the World Food Programme, and “Modelling population distribution and spatial demographic maps” for Africa and Asia for the WorldPop team.

urban-tep.eu



TimeScan Landsat service
(Ostrava and Bohumín)

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POP2

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About the Performance Optimization and Productivity Centre of Excellence in Computing Applications (POP2)

At the end of the year 2018, the POP2 project funded by the European Union Horizon 2020 programme started. It directly follows and extends the activities successfully carried out within the POP Centre of Excellence since 2015. Its primary activities include assistance with analysis of parallel applications, identification of erroneous parts of codes, and recommendations for optimization methods resulting in increased performance and better scalability of a given application.

POP2, coordinated by Barcelona Supercomputing Center (BSC), will continue until November 2021.
The seven following partners will participate in the project implementation: the University of Stuttgart, Forschungszentrum Jülich, and RWTH Aachen University (Germany), Numerical Algorithms Group (UK), the Teratec company and the University of Versailles Saint Quentin-en-Yvelines (France), and IT4Innovations National Supercomputing Center (Czech Republic). The principal investigator for IT4Innovations is Lubomír Říha.

pop-coe.eu

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ExCAPE

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Successful completion of the ExCAPE project aiming at development of computer programmes capable of new drug discovery using exascale computing

New drug design, discovery, and development is a lengthy and costly process. It takes an average of 10 years and costs around EUR 1 billion. The power of exascale supercomputers will allow such time-consuming and finance--intensive laboratory tests to be replaced with more precise, faster, and cheaper computer simulations. The objective of the ExCAPE project, funded by the European Union Horizon 2020 programme for research and innovation, was to design and write computer programs capable of new drug discovery using exascale computing.

Our participation within the project consisted in developing state-of--the-art scalable algorithms and their suitable implementation. The respective algorithms were developed for solving complex problems in pharmacology with respect to processing large amounts of data needed for industrial drug development.

Within ExCAPE, our colleagues developed the HyperLoom software for easy data processing using supercomputers. In 2018, this software even got attention of the European Commission's Innovation Radar initiative aiming to identify European innovators and innovation and to select the finalists for the Best Innovation Competition through public voting.

For an article about the ExCAPE project, please, visit the website of the European Commission "Future and Emerging Technologies" programme: www.fetfx.eu/story/supercomputer-will-discover-future-medicines

For a promotion video of the ExCAPE project, please visit: vimeo.com/256141454

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EURONEWS REPORT

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For more details, see the report using the following link:
www.euronews.com/2019/03/14/supercomputer-supercharging-innovation-in-the-czech-republic

The Euronews television network has filmed a report at our centre

At the beginning of 2019, the pan-European Euronews television network filmed a report at our centre within the Intelligent Regions programme, which aims to bring media coverage to important projects of high value for European Union citizens.

Vít Vondrák, IT4Innovations Managing Director, told Euronews:
"We are trying somehow to help the companies, showing them how to adopt HPC technologies, high performance computing technologies for their businesses. We are providing them experts, we are providing them experience, and we are helping them to adopt such technologies for their businesses."

Tomáš Kozubek, IT4Innovations Scientific Director, told Euronews:
"It is possible to parallelise different computations and therefore accelerate them. It means that if some company needs to do some large computations they are able to run these computations using supercomputers much faster. And this is very important when they develop some new product, because if you want to be innovative you need to be as fast as possible."

Within the reportage, Euronews also visited two companies that our supercomputing centre helps with innovation acceleration, namely the company Invent Medical Group s.r.o. with the development of cranial orthoses, and the company BORCAD cz s.r.o. with the development of train seats.

Aleš Grygar, co-founder and chief designer of Invent Medical Group, explained to Euronews how much time a supercomputer is capable of saving:
"All of our products are 3D data in the computer. Imagine that you are building them in the computer, or drawing them, it will take 8 hours. Using a supercomputer you can generate them within 8 seconds."

Radomír Bělík, BORCAD cz design engineer, told Euronews:
"The main benefits of a supercomputer for us is we know how to change the main structure of seats, how to do reinforcements, how to optimise the welding process, tube thickness or parts of the seat."

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WHERE YOU CAN MEET US AND WHAT WE HAVE BEEN UP TO LATELY

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On Monday 5th March 2019, the **CzechInno Digital Revolution**, was held at our centre, where our colleagues presented their contributions focused, for example, on case studies and HPC as a service via the HEAppE platform. The event hosted 50 participants.

czechinno.cz/digitalni-revoluce-cz/ostrava

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In the middle of March, we participated at **Kariéra PLUS**, a job fair organized by VSB – Technical University of Ostrava. More than 100 companies and 3,000 visitors attended the event.

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Furthermore, **the InnoHPC Steering Committee meeting and partnership meeting** (High-Performance Computing for Effective Innovation in the Danube Region) were held at our centre. The objective of this project is to enable enterprises as well as academic and research institutions in the Danube Region to develop cooperation in high-performance computing at the national level.

Altogehther 25 participants from Slovenia, Austria, Romania, Bulgaria, Serbia, Croatia, Monte Negro, and Hungary were hosted at the meeting.

Completed and continuing tasks were discussed. One of the yielded results of the project is a web platform developed to allow small and medium enterprises remote access to HPC infrastructures. In September and October 2018, the call for participation of companies active in the automotive and electrical engineering industries in pilot testing of this platform was issued. HPC providers, including IT4Innovations, will establish cooperation with selected companies and help them solve their problems.

www.interreg-danube.eu/approved-projects/innohpc

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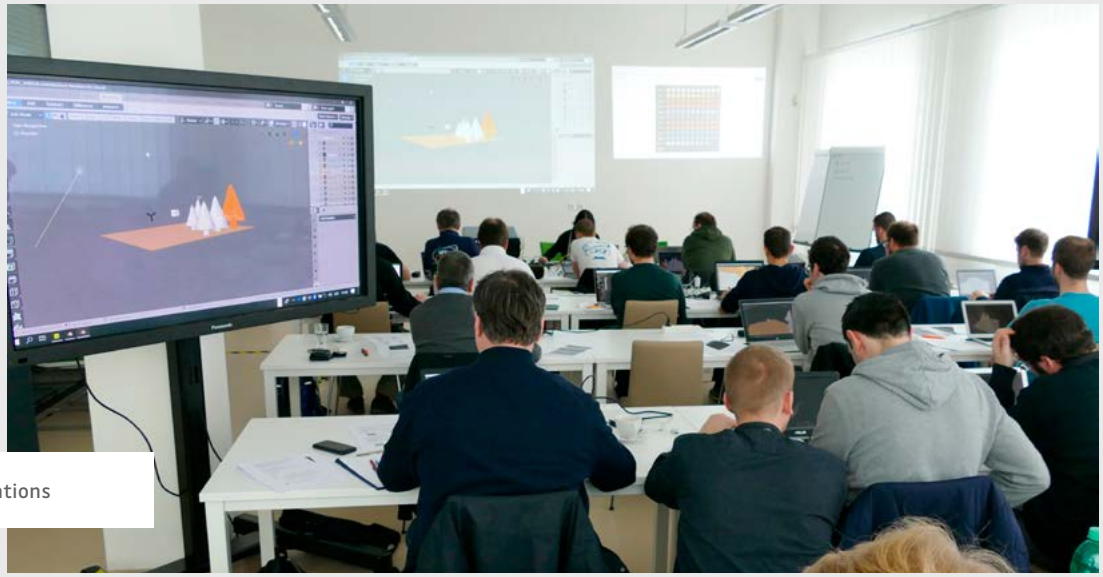
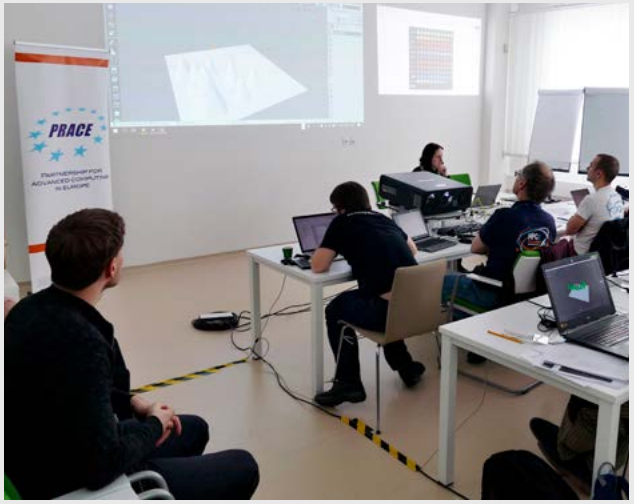
At the end of March, we organized the **Parallel visualization of scientific data using Blender** course, which was completed by 25 participants. The course led by our colleagues Petr Strakoš, Alena Ješko, and Milan Jaroš from the Infrastructure Research Lab was focused on visualization of large datasets generated through simulation of various physical phenomena (e.g., fluid dynamics, structural analysis, etc.). The course participants had an opportunity to get hands-on experience with the Blender software (namely its latest 2.80 version), and the Covise Nodes plug-in for handling scientific data was introduced to them as well. The course ended with rendering a scene on the Salomon supercomputer.

For more about our courses, see training.it4i.cz/kurzy-it4innovations





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