NEWSLETTER Q1/2020

VSB TECHNICAL UNIVERSITY OF OSTRAVA

IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

KRÁTCE

DIH OSTRAVA SET UP

On 30th January 2020, IT4Innovations National Supercomputing Center and the Moravian-Silesian Innovation Centre Ostrava concluded a memorandum establishing the Digital Innovation Hub Ostrava. The strategic objective of DIH Ostrava is to encourage implementation and utilisation of advanced digital innovation across enterprises as well as society.

LUMI END USER WEBINAR

HPC fans are welcomed to participate at the LUMI end user webinar and learn about the functionality of the LUMI research platform and its use to the fullest. The webinar is scheduled for 19th May from 9 am to 11.30 am.

To enrol for the webinar, use the following link

IT4INNOVATIONS SELECTED BY THE EC AS THE COMPETENCE CENTER FOR HPC

The main goal of the HPC Competence Centers (EURO CC) is to systematise support at the European level for the deployment of HPC technologies based on strongly interconnected National Competence Centers (NCCs) to support academia, public administration and industry (especially SMEs) by benefiting from the available expertise, experience and resources of HPC in Europe.

PRIORITY ACCESS TO COMPUTATIONAL RESOURCES

IT4Innovations offers priority access to its computational resources for projects aimed at mitigating the spread of the COVID-19 disease.

For more information, see

TOMÁŠ KOZUBEK FOR THE UNIVERSITAS MAGAZINE

Tomáš Kozubek, the IT4Innovations Scientific Director, responded to the questions asked by Universitas, a magazine for universities, regarding not only IT4Innovations but also the technological level of supercomputers housed by European centres in comparison to the USA and Asia as well as about the overall IT level in Ostrava.
For full article, see

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PROJECT FOR RESEARCH AND DEVELOPMENT OF AN OBSTACLE DETECTION SYSTEM IN RAILWAY TRAFFIC KICKS OFF

Project for research and development of an obstacle detection system in railway traffic kicks off

In January this year our colleagues from the Infrastructure Research Laboratory and the Advanced Data Analysis and Simulations Laboratory started working on a project entitled Research and Development of a Functional Sample of a Railway Vehicle Enabling Collection of Data and Software – a Simulator Enabling Generation of Data to Train Obstacle Detection under Simulated Conditions, which was supported in the 1st open call of TA CR within the TREND programme to support industrial research and experimental development.

During the upcoming three years our colleagues, in cooperation with the IXPERTA s.r.o. company, will be involved in a research project focused on both development of a functional sample of a railway vehicle enabling collection of data using modern sensors, and a software simulator enabling generation of training data for development of an obstacle detection system.

The main objective of the project is to develop a functional sample of a railway vehicle detecting obstacles in the driving profile. In order to do so, a set of HW sensors, a sophisticated architecture for data processing, and artificial intelligence tools for final identification of obstacles and their interpretation to the locomotive driver will be used. 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.

The simulator will enable the creation of a virtual 3D environment of a railway. Moreover, the main sensors being eventually mounted to a real train will also be modelled. A support of sensors such as a video camera, LIDAR, and thermal camera is foreseen. Such an environment will allow simulation of crisis situations, which may analogously arise on a real railway. In addition, it will enable different weather phenomena such as rain, snow, and fog to be simulated and thus generated output data to be affected.

During the simulator development, important potential scenarios will be specified and important susceptible parameters of the virtual environment will be selected in order to define the simulator complexity as well as to ensure the desired variability and credibility of data necessary for training the detection algorithm.

In this project, IT4Innovations is particularly involved in the simulator development. This will include creation of its fundamental concept and subsequent extension of its functionalities. Implementations of different scenarios and each simulation will be progressively improved and enhanced, respectively. Last but not least, the simulator development will also include testing of its functionality as well as of its limits and validation of its outputs.

The Research and Development of a Functional Sample of a Railway Vehicle Enabling Collection of Data and Software – a Simulator Enabling Generation of Data to Train Obstacle Detection under Simulated Conditions project, ID FW01010274, is co-funded with the state aid of the Technology Agency of the Czech Republic within the TREND Programme.

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NEW UPCOMING NVIDIA DEEP LEARNING INSTITUTE COURSES GET THE GREEN LIGHT AT IT4INNOVATIONS

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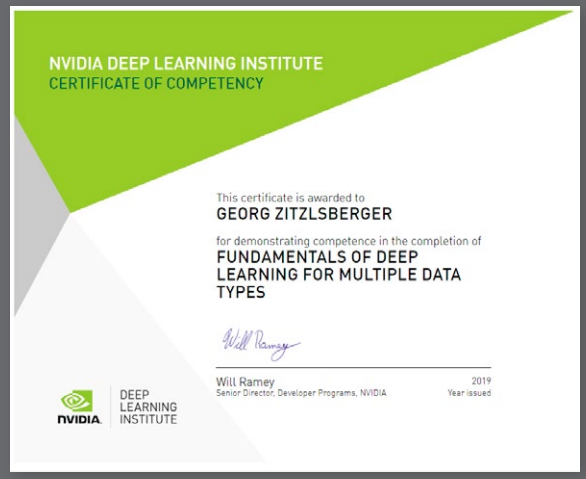
New upcoming NVIDIA Deep Learning Institute courses get the green light at IT4Innovations

Since 2018, IT4Innovations has been the NVIDIA Deep Learning Institute Ambassador. Our colleague Georg Zitzlsberger has obtained two further certificates and our users may thus look forward to participating in other courses focused on Deep Learning and AI.

The NVIDIA Deep Learning Institute offers practical courses for developers and scientists who would like to solve complex problems using Deep Learning. The institute is focused on teaching the latest methods for design, learning, and implementation of machine learning based on neural networks in various research and application areas via its NVIDIA certified courses. Course participants have an opportunity to become familiar with widely used open-source tools and the latest Deep Learning platforms accelerated by NVIDIA graphical processors in practice.

In 2018, Georg Zitzlsberger was awarded the Fundamentals of Deep Learning for Computer Vision certificate and is newly a holder of the Fundamentals of Deep Learning for Multiple Data Types and Fundamentals of Deep Learning for Multi-GPUs certificates.

NVIDIA | DEEP LEARNING INSTITUTE


NVIDIA DEEP LEARNING INSTITUTE
CERTIFICATE OF COMPETENCY

This certificate is awarded to
GEORG ZITZLSBERGER

for demonstrating competence in the completion of
FUNDAMENTALS OF DEEP LEARNING FOR MULTIPLE DATA TYPES

Will Ramey
Senior Director, Developer Programs, NVIDIA

2019
Year issued

NVIDIA DEEP LEARNING INSTITUTE

Certification NVIDIA DEEP LEARNING INSTITUTE

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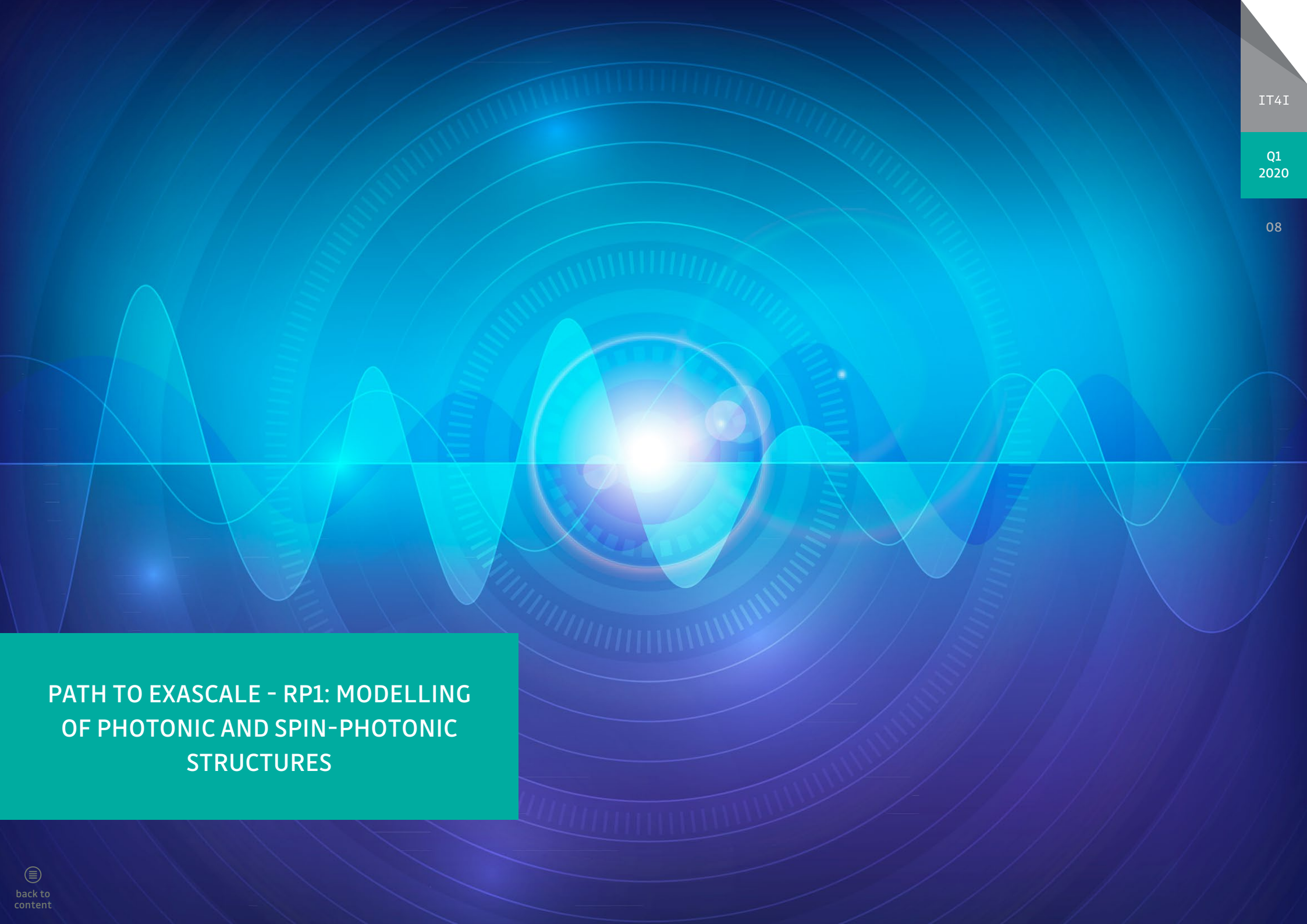

PATH TO EXASCALE - RP1: MODELLING OF PHOTONIC AND SPIN-PHOTONIC STRUCTURES

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Path to Exascale - RP1: Modelling of Photonic and Spin-photonic Structures

The IT4Innovations National Supercomputing Center – Path to Exascale project is focused on modernization of the IT4Innovations research infrastructure and development of its in-house research in order to maintain a high technological level of HPC in the Czech Republic primarily in comparison with European countries. The project has been running since 2017 and shall be completed in 2021. Within this project, the in-house research has been conducted via three research programmes.

In this Newsletter, we are presenting Research Programme 1: **Modelling of photonic and spin-photonic structures**, which is focused on materials with magnetooptical activity, new sources for terahertz radiation, and modelling of photonic and spin-photonic structures.

Magnetooptical Materials

The optical anisotropy of magnetooptical materials is a function of magnetisation M, and, thus, also function of external magnetic fields. Linearly polarized light becomes elliptically polarized upon reflection from a magnetized specimen (Fig.1). This phenomenon is the well known magnetooptical Kerr effect (MOKE), which can be utilized, for example, in research of ferromagnetic materials, which are the backbone of high-capacity hard drive disks. It can also be used in detection of spintronic and spincaloritronic phenomena.

One of the achievements of the team from the IT4Innovations Modelling for Nanotechnologies Laboratory in this field has been the development of quadratic MOKE (QMOKE), being the contribution in the second order in magnetization to the overall MOKE signal, i.e. part of MOKE proportional to M2. QMOKE is not only crucial for correct interpretation of all MOKE signals but also for characterization of antiferromagnetic materials. These materials could possibly be the future of the data storage industry. Our team has achieved success in the development and application of a novel QMOKE spectroscopy technique which allows a QMOKE contribution to be separated from the linear part of MOKE, and its origin in the permittivity tensor of MO material to be determined in the visible spectral range with the overlap in the UV and IR part of the spectra. Such experimentally obtained data can then be described using ab-initio theoretical calculations where use of HPC is often a necessity. The research was presented in an article by R. Silber et al. entitled Quadratic Magneto-optic Kerr Effect Spectroscopy of Fe Epitaxial Films on MgO (001) Substrates, published in Phys. Rev. B 100, 064403 (2019).

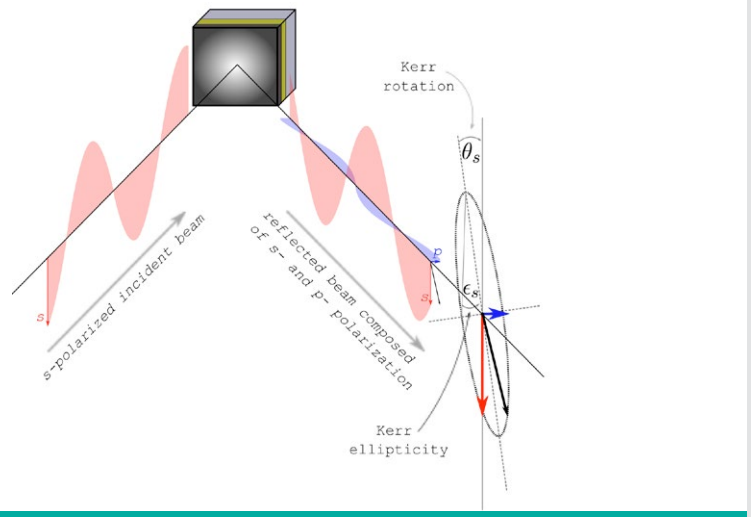

Fig 1: Linearly s-polarised light, after being reflected from a magnetooptical material, becomes elliptically polarised, which is an effect described by Kerr rotation and ellipticity.

PATH TO EXASCALE PROJECT

Research programme RP 1 – Modelling of Photonic and Spin-photonic Structures
Principal investigator: Prof. Jaromír Pištora
Research programme RP 2 – Design of New Materials Based on Ab Initio Electronic Structure Calculations
Principal investigator: Dr Dominik Legut
Research programme RP 3 – Analysis of Image Data Using HPC
Principal investigator: Dr Pavel Tomančák

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New sources for Terahertz Radiation

Terahertz (THz) radiation is part of the electromagnetic waves spectrum with a wavelength ranging from approximately 0.1 to 1 mm. It has a wide range of applications such as high-speed wireless communication, security scanners (e.g. at airports), astrophysics, and material characterisation. At IT4Innovations, we design sources and detectors of THz radiation. One achievement includes development of the NH3 molecular THz laser. The results were published in a paper by M. Mičica et al. entitled High-resolution THz Gain Measurements in Optically Pumped Ammonia, published in Optics Express, 26, 21242-21248, (2018).

Modelling of Photonic and Spin-photonic Structures

(Spin-)photonic structures include, for example, the spin-vertical-cavity surface-emitting laser (spin-VCSEL). VCSELs are fundamental devices in high-speed optic communication. At IT4Innovations, we are involved in design and optimisation of spin-VCSELs, i.e. lasers using not only electron charge but also electron spin to generate light (Fig. 2). Design and optimisation of these structures are computationally intensive, and thus use of HPC is a necessity. Therefore, the application of spin-VCSELs in optic communication is promising for a significant increase in data transfer speed as presented in a paper by T. Fördös et al. entitled Muller Matrix Ellipsometric Study of Multilayer Spin-VCSEL Structures with Local Optical Anisotropy, published in App. Phys. Lett. 112, 221106 (2018).

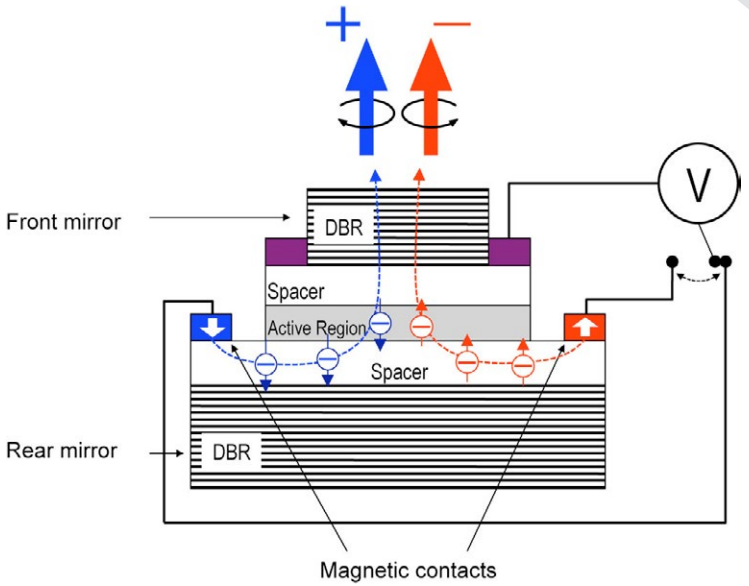

Fig. 2: Spin-VCSEL structure scheme. The active part of the laser is enclosed between two mirrors (DBR = Dielectric Bragg Reflector). Polarisation of the generated light is then dependent on pumping electron spins.

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

MINISTRY OF EDUCATION, YOUTH AND SPORTS

This work was supported by the European Regional Development Fund from the IT4Innovations national supercomputing center – path to exascale project (CZ.02.1.01/0.0/0.0/16_013/0001791) implemented within the OP RDE.

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URBAN TEP PLATFORM

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Urban TEP Platform

In 2014, the European Space Agency (ESA) started the Earth Observation Exploitation Platforms (EPs) initiative, which integrates a set of research and development activities aimed at development of an ecosystem of interconnected Thematic platforms - TEPs. These platforms include Coastal TEP, Forestry TEP, Geohazards TEP, Hydrology TEP, Polar TEP, Urban TEP, and Food Security TEP.

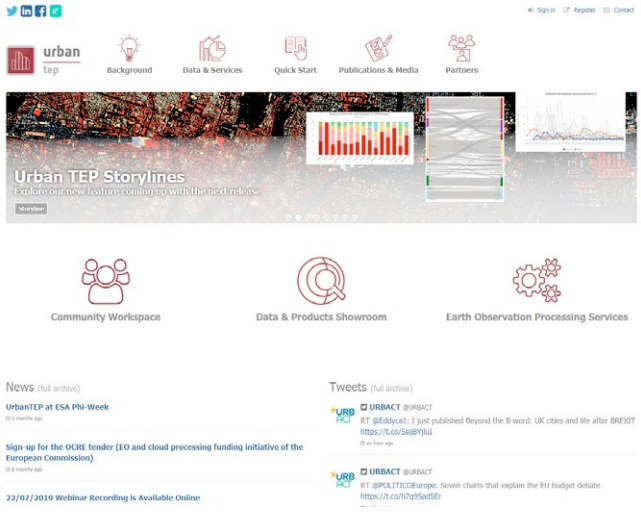
Urban TEP aims to use functions and services of modern information technologies in order to bridge the gap between the technologically driven Earth observation sector and environmental science, planning, and policy needs. The key component is an open web portal connected to distributed high-level computing infrastructures providing key functionalities for access to data, their processing, analysis, and visualization along with an option for customised development and sharing of algorithms, products, and services via dedicated networking and communication tools.

Case studies and analyses include, for example, creation of cloud-free mosaics, which provide a consistent spatio-temporal view of urban environments and the adjacent land, generation of global poverty-related indicators, quantification of regional land use dynamics in Asian urban areas, and derived orthomosaics and digital surface models from drone-generated data, among others.

The main activity of IT4Innovations in this project is to provide state-of-the-art technology and expertise in high-performance computing, i.e. processing and storage of data needed for access, analysis, and visualization of geospatial data and derived products. In 2019, the Urban TEP project entered a new stage focused on systematic improvement and streamlining of the platform capabilities and functionalities as well as on development of tailored products and services.

Having an innovative character, the Urban TEP platform has already attracted a huge user community. More than 300 institutions from more than 40 countries (scientific and public institutions, non-governmental organizations, industrial enterprises, etc.) have requested access to products and services offered by the Urban TEP platform so far.

The objective of Urban TEP is to open up new opportunities to facilitate efficient and effective urban management and protection of residents by systematically exploring unique EO (Earth observation) capabilities in combination with a big data perspective arising from ever growing sources of geodata.



Web platform Urban TEP

THEMATIC EXPLOITATION PLATFORM (TEP)

TEP is a collaborative virtual work environment with one coherent user interface which provides access to EO (Earth Observation) data and tools, processors, and resources essential for processing and storage of data needed for efficient extraction, analysis, and visualisation of thematic geoinformation from mass EO (Earth Observation) data sources. For more about the platform, see

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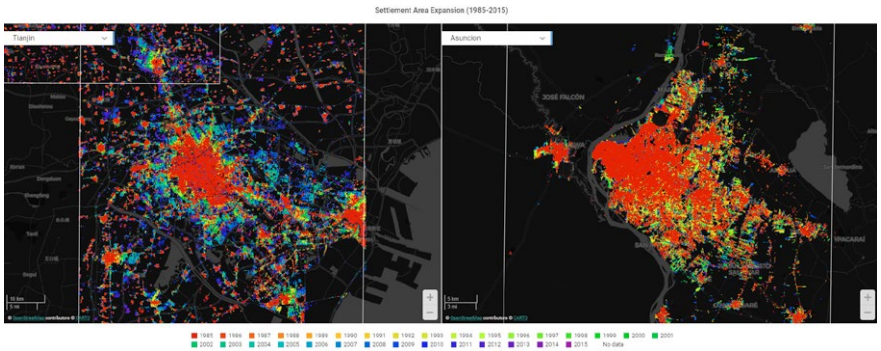
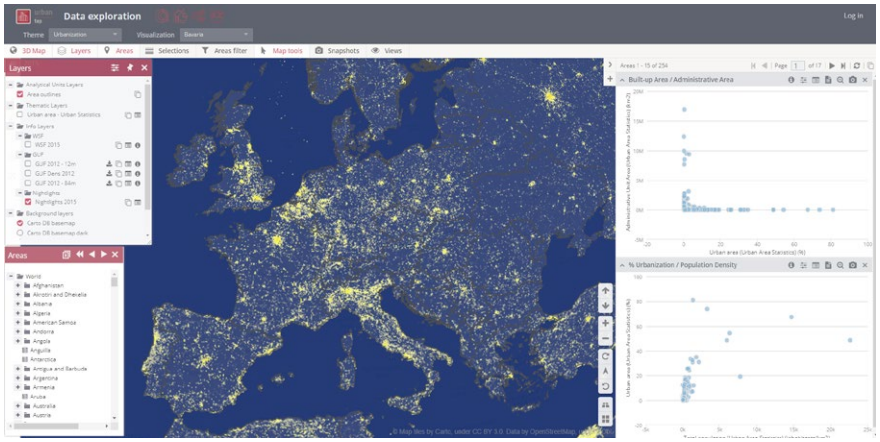


Extension of a populated area



Night-time light data research

URBAN TEP CONSORTIUM

The UrbanTEP platform is operated by an international consortium consisting of five partners:

- German Aerospace Center (Germany)
- Brockmann Consult GmbH (Germany)
- Terradue Srl (Italy)
- IT4Innovations (Czech Republic)
- Gisat s.r.o. (Czech Republic)

DLR Deutsches Zentrum für Luft- und Raumfahrt German Aerospace Center · Brockmann Consult · terradue · VSB Technical University of Ostrava | IT4Innovations National Supercomputing Center · gisat

esa

The Urban Thematic Exploitation Platform (U-TEP) project was supported by the European Space Agency (ESA), as a sub-project of the German Aerospace Center ID No. D/565/67215517.

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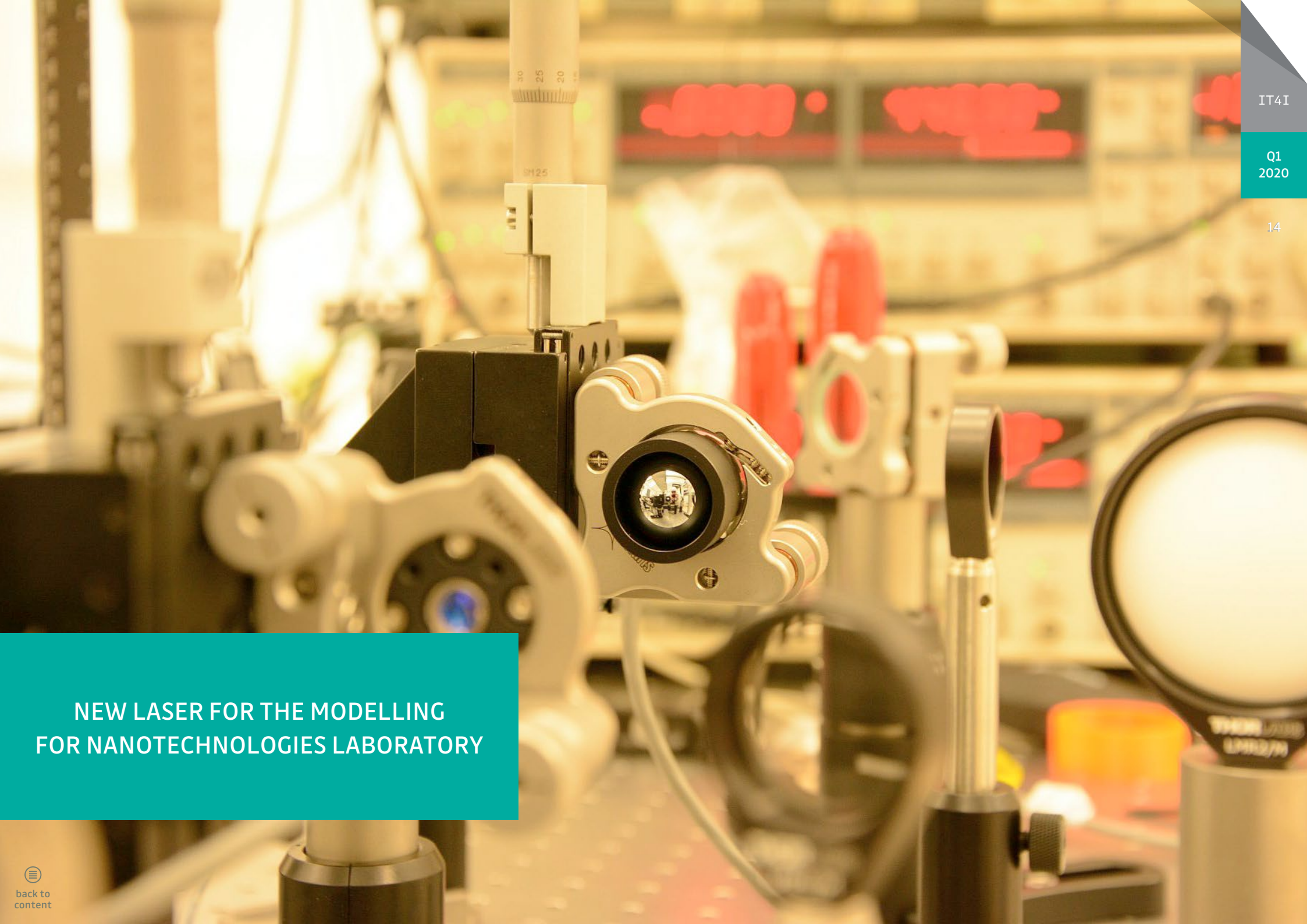

NEW LASER FOR THE MODELLING FOR NANOTECHNOLOGIES LABORATORY

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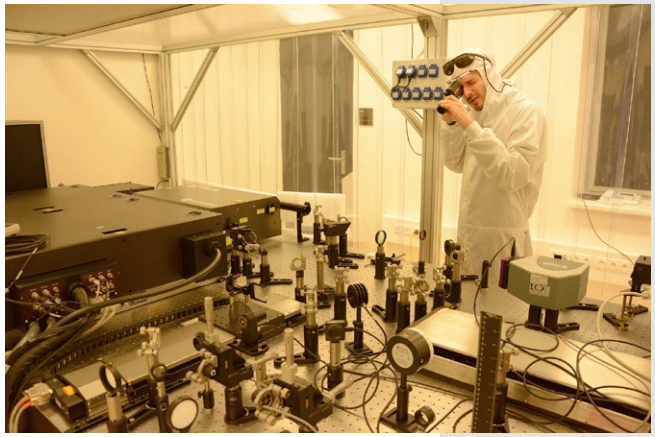
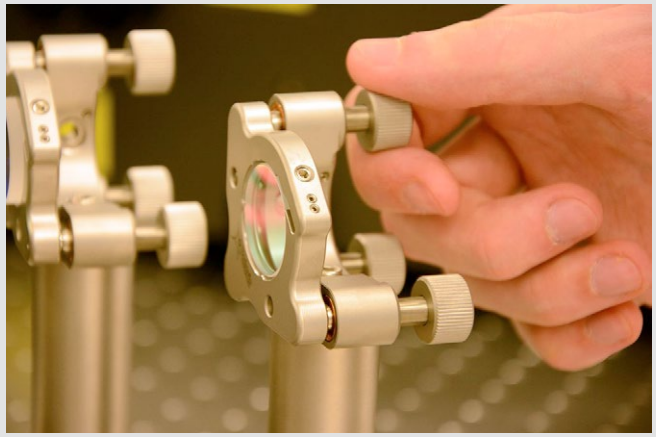
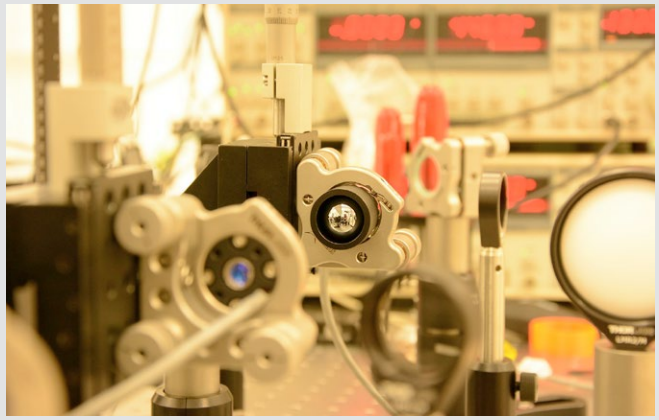
New laser for the Modelling for Nanotechnologies Laboratory

The modernized laboratory for research activities of the IT4Innovations Modelling for Nanotechnologies Laboratory is equipped with a specialized laser for generation of ultrashort femtosecond pulses, i.e. laser beams with duration of a quadrillionth of a second (10^{-15} s).

Ultrashort femtosecond pulses are shorter in terms of their duration than the length of a huge number of elementary physical, chemical, and biological processes on a molecular level. Using these ultrashort pulses, the laboratory team can observe the dynamics of the above-mentioned processes in time. Another advantage is the aggregated performance per pulse, which exceeds the performance of a nuclear power plant by several orders of magnitude despite having little energy per pulse (in mJ). In the interaction of a pulse with studied matter, the research team will be able to generate special states of matter and explore the processes, during which light reacts with matter in a different manner than we are used to. Experiments will be based on pump-probe ellipsometry, magnetooptics, terahertz time-domain spectroscopy, and two-photon polymerization 3D printing.







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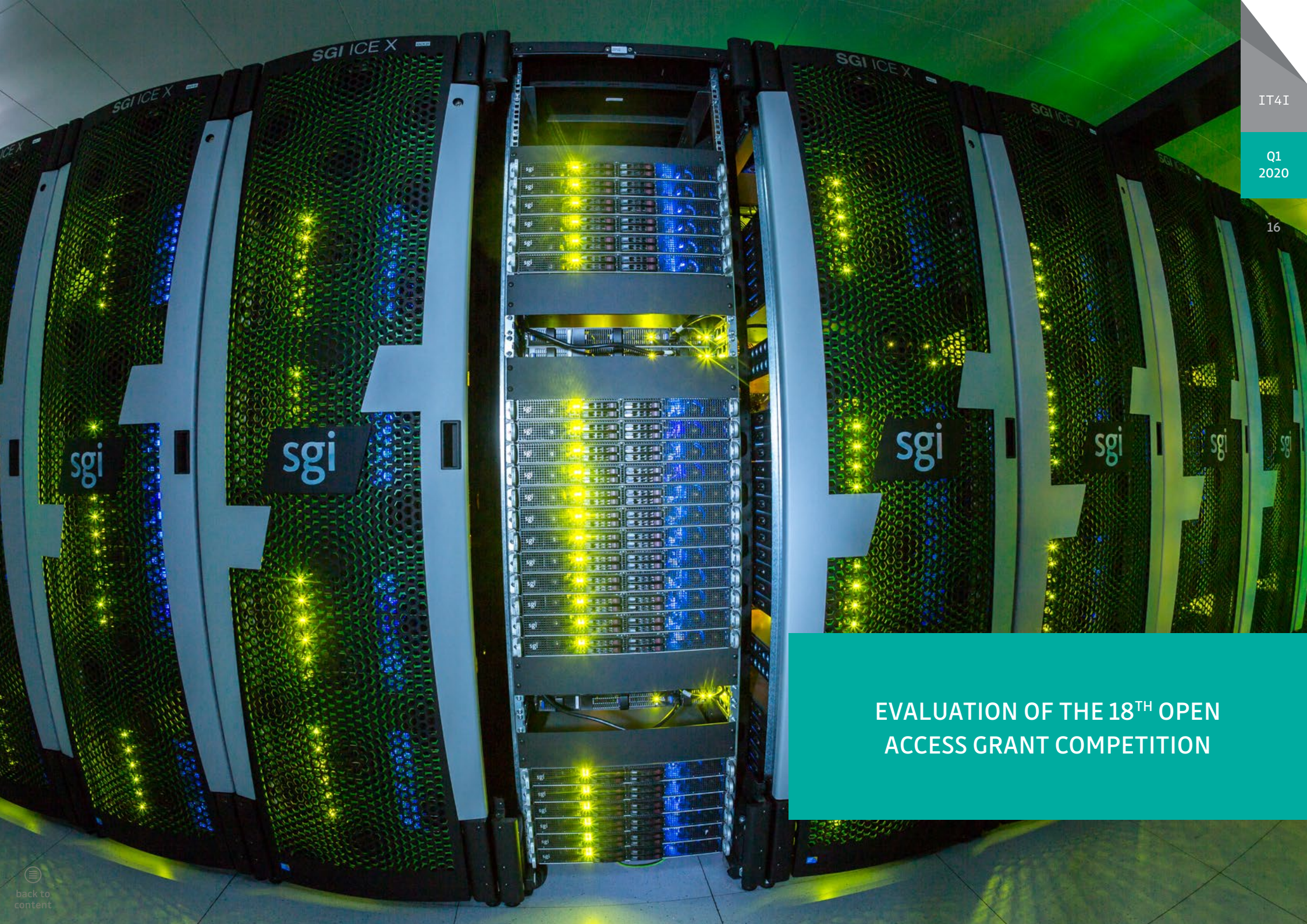

EVALUATION OF THE 18TH OPEN ACCESS GRANT COMPETITION

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Evaluation of the 18th Open Access Grant Competition

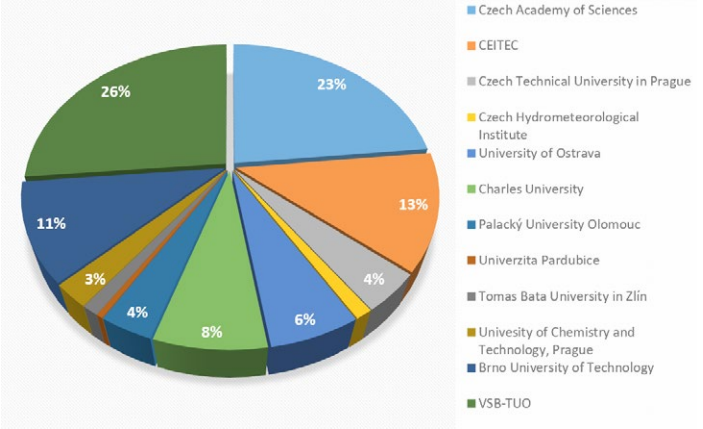
In the 18th Open Access Grant Competiton, within the standard 9-month access, interested users applied for more than 137 million core hours. The required resources exceeded the capacity of 85 million core hours by 61 %. With respect to high demand in the computational resources, the allocation committee decided to decrease the initial allocation for each individual project. In this Open Access Grant Competition, the allocation committee have thus distributed 85 million core hours across 60 successful projects, with 8 of them being multi-year projects.

The majority of core hours, specifically 20 million (i.e. 26 % of the total distributed computational resources), were awarded to researchers from VSB-TUO for 12 projects. Institutes of the Czech Academy of Sciences were awarded more than 18 million core hours (i.e. 23.3 % of the total distributed computational resources) for 19 projects, and CEITEC as a research centre of Masaryk University was awarded 9 million core hours (i.e. 13 % of the total distributed computational resources).

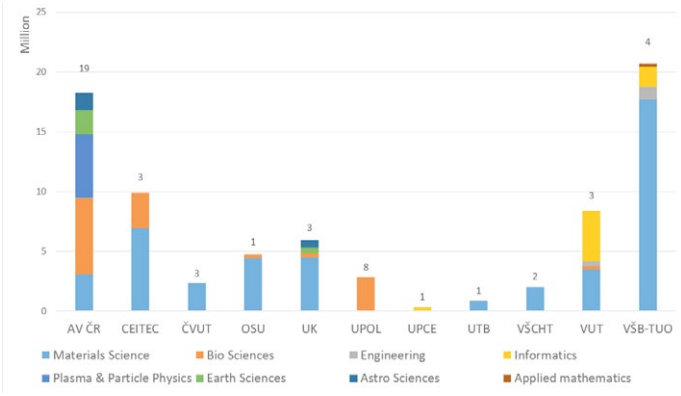
Other institutions awarded the computational resources for implementing their research projects in the 18th Open Access Grant Competition include CTU and Charles University in Prague, the University of Ostrava, Brno University of Technology, the University of Chemistry and Technology in Prague, Palacký University in Olomouc, the University of Pardubice, the Czech Hydrometeorological Institute, and Tomas Bata University in Zlín.

Allocation of computational resources in the 18th Open Access Grant Competition by research domains and organizations

Allocation of more than 1 million core hours was awarded to 22 projects of researchers from Charles University in Prague, the Czech Technical University in Prague, the Czech Academy of Sciences, Masaryk University, the University of Ostrava, Brno University of Technology, Palacký University in Olomouc, and VSB – Technical University of Ostrava. The first three most successful projects were awarded a total amount of 19 million core hours. Almost 7 and approximately 6 million core hours were awarded to Dominik Legut from IT4Innovations for his project entitled Strengthening and Toughening w-BN by 3D Networks of Planar Defects and Mojmír Šob 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.



Allocation of computational resources in the 18th Open Access Grant Competition within the standard 9-month access



Allocation of computational resources in the 18th Open Access Grant Competition by research domains and organizations

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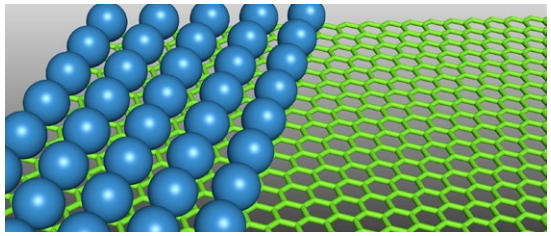
LET US INTRODUCE SOME OF THE AWARDED PROJECTS:

Dr Matúš Dubecký
University of Ostrava
ACCURACY LIMITS OF QUANTUM MONTE CARLO IN WEAK-INTERACTION LIMIT III

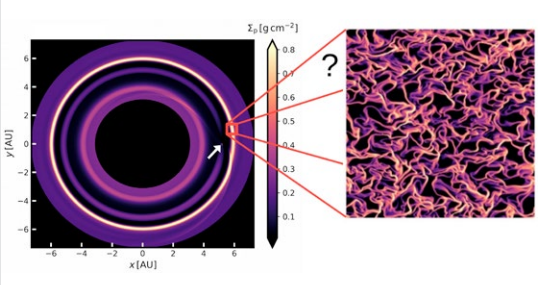
More than 4 million core hours were awarded to Matúš Dubecký for his research focused on determining the accuracy limits of the Fixed-node diffusion Monte Carlo (FNDMC) method for noncovalent interactions. Noncovalent interactions play a key role in many research areas such as material science and drug design. The team led by Matúš Dubecký will conduct a benchmark study as a follow up to their previous research and application of the FNDMC method, for example, in 2D materials, the properties of which are affected by noncovalent interactions of molecules, and 1D conductors on their surfaces. The objective of this project is to determine, by means of a supercomputer, the accuracy limits of the FNDMC method, which is currently frequently used as a quantum reference method for large noncovalent systems. Apart from gaining a physical insight into the FNDMC method and design of potential improvements, the results will lead to better accuracy control and more rational application of this method not only for large systems.



Visualization of an adsorbed argon monolayer on graphene

Dr Ondřej Chrenko
Astronomical Institute of Charles University in Prague
PLANET FORMATION AFTER PEBBLE ISOLATION

Ondřej Chrenko was awarded more than 600,000 core hours for his project focused on planet formation processes. Modern scenarios of planet formation suggest that planets form by accretion of cm to m-sized solid particles, the dynamics of which is subject to the aerodynamic drag in the surrounding protoplanetary disk. The drag not only causes a radial drift of pebbles through the disk but also enhances the efficiency of the gravitational capture of pebbles by a planetary embryo. However, once the mass of a growing protoplanet exceeds a certain threshold, a pressure bump is formed in the gas outside the planetary orbit where pebbles start to accrete, and the protoplanet growth ceases. The objective of this project is to investigate the evolution of pebbles, which gradually accumulate in the pressure bump. Ondřej Chrenko will use the IT4Innovations supercomputers for 2D and 3D simulations of a two-fluid flow (solid-to-gas) system in order to verify if hydrodynamic instabilities occur in the pressure bump. These instabilities might cause pebbles to become concentrated into clumps, which might undergo a gravitational collapse, thus forming a new planetary embryo. Using local, high-resolution simulations, the project team will study whether hydrodynamic instabilities, such as those in the figure on the right (Comment: the figure on the right is borrowed from a paper by Benítez-Llambay et al. 2019), may occur in the pressure bump.



Pebble concentration (in surface density units) in the part of the protoplanetary disk with an embedded 30 Earth mass protoplanet. The planet location is highlighted by the arrow. The length unit on the x and y axes, i.e. 1 au, corresponds to the distance between the Earth and the Sun.

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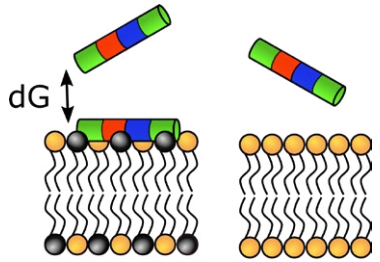
Dr Robert Vácha
CEITEC

PROTEIN AFFINITY AND SELECTIVITY TO CELLULAR MEMBRANES

For the first phase of his research focused on protein affinity and selectivity of cellular membranes, Robert Vácha was awarded almost 2.9 million core hours. Spatial and temporal organisation of proteins in the cell is a crucial aspect for understanding the complex processes in living cells. Peripheral proteins organised at membranes of specific organelles to correctly perform their functions are important elements. However, the relationship between the protein sequence and its membrane is not yet known. The aim of the proposed project is to identify, quantify, and explain protein affinity for membranes with specific lipid composition. The team led by Robert Vácha aims at developing a computational method to determine the finding free energy of proteins and their mutants to membranes with specific lipid composition. Application of this method with the aid of the IT4Innovations computational resources will provide molecular understanding allowing the preferred localization of proteins in cells to be determined and as such it can be used in development of new protein biomarkers, sensors, and drugs.

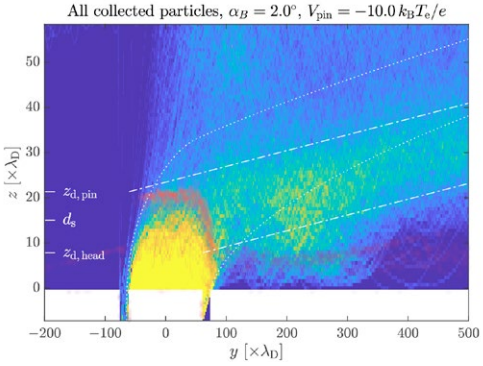


The amphiphilic peptide with affinity strongly dependent on the specific lipid composition of membranes.

Dr Aleš Podolník
Institute of Plasma Physics of the CAS

SIMULATION OF PROBE DIAGNOSTICS FOR COMPASS-UPGRADE

Aleš Podolník was awarded more than 1 million core hours for simulation of probe diagnostics for the COMPASS-U tokamak, a world-class fusion research facility which is currently being designed and constructed. This device shall produce plasmas relevant to those ones in the future ITER and DEMO fusion reactors. One of the planned areas of research is also to design plasma facing components, which require complex diagnostics equipment. To study the unique plasma properties in the COMPASS-U tokamak, both the existing and the newly-developed diagnostics systems will be used. One such diagnostic is Langmuir probes which, when properly set up, can measure electron temperature and density essential for calculation of thermal stresses of the plasma facing components. However, design and use of probes for measurements inside the tokamak with extreme plasma parameters takes significant effort. The research project of Aleš Podolník and Michael Komm aims at simulation of probes that would be accommodated to various variants as well as shaping options of plasma facing components inside the tokamak. Previous research projects show that proper probe design is crucial not only from the operational point of view, for example, to avoid melting of the probe under extreme plasma energy flow, but also to maximize the accuracy and precision of obtained physical data, in particular.



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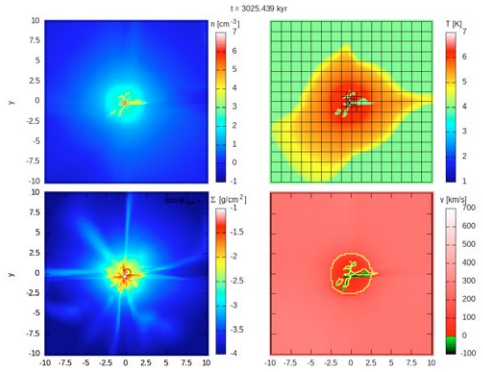
Dr Michail Kourniotis
Astronomical Institute of the CAS

IMPACT OF MASSIVE STARS ON THE COMPOSITION OF GLOBULAR CLUSTERS

Michalis Kourniotis from the Astronomical Institute of the CAS was awarded 718,000 core hours to study the impact of massive stars on the composition of globular clusters. With a diameter of tens of light years, globular clusters are spheroidal dense collections of hundreds of thousands to millions of very old stars. They can typically be found in the spheroidal halo of the Milky Way and other galaxies. Originally thought to comprise of stars of the same age, it is now well established that globular clusters host multiple generations of stars with different ages and chemical compositions.

Numerical methods for simulating the non-stationary wind of massive clusters are valuable for acquiring knowledge about gas dynamics inside a small globular cluster and thermal instabilities that potentially lead to newborn stars, in particular. The latest stellar evolutionary models provide essential input parameters to determine the mass and energy accumulated in globular clusters by massive stars in the form of extremely fast stellar winds and supernovae outbursts.

Michail Kourniotis with his colleagues Richard Wünsch and Barnabás Barna will use the supercomputer to perform high-resolution 3D simulations to obtain information about formation of several stellar generations in spheroidal globular clusters. In addition, the objective of this project is also to study the impacts of extreme stellar types on the wind evolution in globular clusters and its spatial distribution.

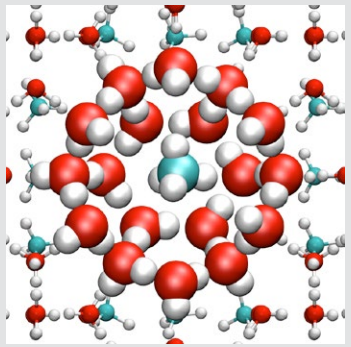


High-resolution hydrodynamic simulation of gass in a massive globular cluster (up to 512^3 cells). The 10^7 sollar mass globular cluster is 3 million years old, and its chemical composition is typical for a young universe. Each panel shows the logarithm of gas particle density (n), temperature logarithm (T), column density of gas logarithm (Σ), and gas flow speed. The circle denotes the site where new stars form.

Dr Jiří Klimeš
Charles University in Prague

ACCURACY AND PRECISION FOR EXTENDED SYSTEMS IV

More than 2.8 million core hours of the IT4Innovations computational resources were awarded to a team led by Jiří Klimeš for a project focused on precision and accuracy of binding energies calculations in crystals, especially those bound by non-covalent interactions. These materials, such as methane clathrates at the bottom of the sea, pharmaceuticals crystals, and layered systems such as graphite to name but few. One of their peculiar properties is polymorphism – the ability of a crystalline material to adopt different crystal structures, even under same conditions. One of the objectives of this project is to use a supercomputer to develop a method that would allow a reliable description of the stability of different polymorphs or different crystalline phases of materials. It is a basic research project aiming at both gaining deeper understanding of the accuracy limits of the currently used methods and development of higher precision methods applicable in future material simulations. The research team led by Jiří Klimeš would also like to integrate developed scripts for preparation and analysis of calculation into "packages" used for automated working procedures. This all is expected to ensure that the methods for accurate calculations of binding energies can be used by other research groups as well as increase reproducibility of such results.



In methane clathrate, the methane molecules are surrounded by water molecules. A reliable calculation of their mutual interaction requires application of high-precision methods.

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WE ARE SOLVING ANOTHER EUROPEAN SPACE AGENCY (ESA) PROJECT – BLENDED

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Blockchain ENabled DEep Learning for Space Data (BLENDED)

In January 2020, our colleagues from the IT4Innovations Advanced Data Analysis and Simulations Laboratory started their work on the Blockchain ENabled DEep Learning for Space Data (BLENDED) project, which was announced within the Open Call of the European Space Agency (ESA).

There are four other partners together with IT4Innovations implementing the project, the objective of which is to evaluate technologies allowing secure, valuable, and efficient interconnection of data and technologies. Namely, it includes the use of Inter-Planety File System (IPFS) protocol, encryption, and the Blockchain smart contract technology. Such combination of technologies shall lead to the development of a prototype of a distributed peer-to-peer platform using machine learning to analyse space data, including monitoring of the data and algorithms ownership and prevention of their unauthorised use.

The project will aim to use neural networks for a case study: Analysis and prediction of time series to monitor the growth of urban agglomerations using Earth Observation data. To train neural networks, for three selected cities, different sources of satellite as well as non-satellite data will be used. The selected cities include: Limassol (Cyprus) – in comparison with 20 years ago, the local urban agglomeration has tripled mainly due to tourism and the oil and gas industry, Liège (Belgium) – a city with a rich industrial tradition situated in the vicinity of Brussels, and Rotterdam (Netherlands) – a port with considerably built up urban and industrial areas.

In this project, IT4Innovations is in charge of developing a Deep Learning model aimed at processing remote Earth observation data in order to analyse and predict the growth of urban agglomeration in the monitored cities.

The Synergetic use of Blockchain and Deep Learning for Space Data project (SpaceApps Subcontract No. 4000129481/19/I-IT4I) has been funded by the European Space Agency (ESA) programme.

BLENDED PROJECT

- **5 partners:** Space Application Services (Belgium), Geosystem Hellas (Greece), FORTH (Greece), Faculty of Information Technologies from Brno University of Technology and IT4Innovations (Czech Republic)
- **Implementation period: 1.5 years**
- **Budget: EUR 400,000**

DEEP LEARNING

Deep Learning is part of a broader family of machine learning methods based on artificial neural networks with representation learning. Learning can be supervised, unsupervised, or semi-supervised. Deep learning architectures such as deep neural networks, recurrent neural networks, and convolutional neural networks have been applied to fields including computer vision, speech recognition, natural language processing, audio recognition, social network filtering, machine translation, bioinformatics, drug design, medical image analysis, material inspection, and board game programs, where they have produced results comparable to and in some cases surpassing human expert performance.

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INTERPLANETARY FILE SYSTEM PROTOCOL (IPFS)

InterPlanetary File System protocol (IPFS) is a protocol and peer-to-peer network for storing and sharing data in a distributed file system. IPFS uses content-addressing to uniquely identify each file in a global namespace connecting all computing devices. IPFS allows users to not only receive but also to host content in a similar manner to BitTorrent. As opposed to a centrally located server, IPFS is built around a decentralized system of user-operators who hold a portion of the overall data, creating a resilient system of file storage and sharing.

BLOCKCHAIN

Blockchain is an ever growing list of records, called blocks that are linked using cryptography. Each block contains a cryptographic hash of the previous block, a timestamp, and transaction data. By design, a blockchain is resistant to modification of data. It is an open, distributed ledger that can record transactions between two parties efficiently and in a verifiable and permanent way. Once recorded, the data in any given block cannot be altered retroactively without alteration of all subsequent blocks, which requires consensus of the network majority. Blockchain was invented in 2008 to serve as a public transaction ledger of the bitcoin cryptocurrency. The bitcoin design has inspired other applications and blockchains that are readable by the public and are widely used by cryptocurrencies, in particular.

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NVIDIA AI & HPC ACADEMY 2020

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NVIDIA AI & HPC ACADEMY 2020

At the beginning of February, the unique NVIDIA AI & HPC ACADEMY for all fans of artificial intelligence (AI) and high performance computing (HPC) took place at IT4Innovations. It was a series of hands-on courses organized by the NVIDIA Deep Learning Institute, which made its participants familiar with optimal design and implementation of artificial intelligence problem algorithms on supercomputers. IT4Innovations hosted nearly 90 course participants including representatives from both academia and the commercial sector. The event was supported by NVIDIA, M Computers s.r.o., and PRACE, the pan-European research infrastructure.

Being the holder of the NVIDIA Deep Learning Institute certificate, IT4Innovations is entitled to organize AI-focused courses. In 2019, three such courses attracting enormous interest took place. Therefore, we decided to organize the multi-day NVIDIA AI & HPC ACADEMY. The first day was dedicated to introducing the latest developments in the utilization of the IT4Innovations infrastructure and NVIDIA technologies designated for both research and industry, as the entire event was actually dedicated to these two target groups.

The second day featured the Fundamentals of Deep Learning for Computer Vision course led by Georg Zitzlsberger. A unique aspect of this course was its free entry for representatives from the commercial sector. During the course, the participants learned about deep learning methods for a wide range of computer vision problems including training and deployment of neural networks. *"We really appreciated the opportunity to participate at this event. It is quite a unique and, in fact, unprecedented thing to find such a course open to the commercial sector and, what is more, for free. Generally, it is very difficult to find any Deep Learning-focused courses in the Czech Republic. Availability of such workshops, which are mainly online or take place abroad, is very poor. Therefore, we are enormously happy to be here today,"* commented Tomáš Špacír of the TINT s.r.o. company and one of the participants.

The third and the fourth day featured the Fundamentals of Accelerated Computing with CUDA C/C++ and OpenACC courses designated for participants from academia. Both courses were organized with the support of pan-European research infrastructure PRACE (Partnership for Advanced Computing in Europe) intergrating European supercomputing centres. IT4Innovations is one of the PRACE Training Centres and course lecturers often include renowned experts from all over Europe. Our invitation to the NVIDIA AI & HPC Academy was accepted by colleagues from the Bavarian Leibniz Computing Centre (LRZ), Volker Weinberg and Momme Allalen.

Have a look at the full image gallery of AI & HPC ACADEMY 2020

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WE ASKED VOLKER WEINBERG, A CERTIFIED LECTURER OF THE NVIDIA DEEP LEARNING INSTITUTE (DLI) OPENACC, A FEW QUESTIONS.

Can you describe the collaboration between the Leibniz Computing Centre (LRZ) and IT4Innovations?

"Our collaboration started in 2016 by establishing the Czech-Bavarian Competence Centre for Supercomputing Applications (CzeBaCCA) to foster the Czech-German collaboration in high performance computing. After the termination of the CzeBaCCA project, we continued collaborating within PRACE (Partnership for Advanced Computing in Europe)."

How difficult is it to get certified to lead NVIDIA Deep Learning Institute courses?

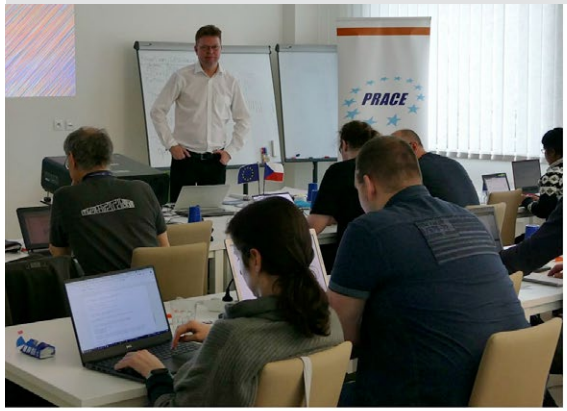
"To get certified as the NVIDIA University Ambassador, I had to pass an interview as well as give a rehearsal lecture at the GTC conference in Munich in October 2018. My colleague Momme Allalen had to take part in several video calls with NVIDIA Deep Learning Institute colleagues in the USA to get certified."

How do you rate the knowledge and involvement of the participants?

"We were very pleased about the great interest and commitment of the participants. It was fun to both teach people who are so dedicated and answer many interesting and challenging questions."

Do you think the OpenACC, CUDA, and OpenMP platforms will coexist together in the future to accelerate computations on GPUs?

"New technologies always come and go and thus it is very hard to predict their future. Using CUDA, you get the best performance on NVIDIA GPU, but with OpenACC and especially OpenMP you can write portable codes, on the other hand. In 2017, OpenMP celebrated the 20th anniversary of its incorporation as well as the release of the first OpenMP API specification for parallel processing. As an LRZ representative in the OpenMP Architecture Review Board, I hope that compiler vendors will increase the OpenMP performance on GPUs and make it future-proof."



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ULRICH MICHAELIS, THE BUSINESS DEVELOPMENT MANAGER FOR NVIDIA HPC SUPERCOMPUTING CENTRAL EUROPE ALSO GRABBED THE OPPORTUNITY TO ATTEND NVIDIA AI & HPC, SO WE ASKED HIM A FEW QUESTIONS AS WELL:

How do you rate the entire event from the perspective of one of the NVIDIA AI & HPC Academy partners?

"It is a great surprise for me how many people from both academia and the private sector participated at this event. I have to admit that this fact has certainly exceeded my expectations. I am happy about our cooperation with IT4Innovations, because it is clearly obvious that IT4Innovations places immense emphasis on education focused on the utilisation of novel technologies. As a producer of new technologies, it is to our delight that people have thus a great opportunity to become familiar with more efficient and appropriate use of these technologies. IT4Innovations and the M Computers company are our great partners in this mission. We help IT4Innovations, in return, with the certification of lecturers, and I personally believe that our partnership is beneficial for all of us."

Do you think such events might continue with next year's edition?

"I certainly do. I think we should continue with our efforts and make it a tradition as technologies are constantly evolving. Such events are great for many reasons. Firstly, it is a great opportunity for representatives from both academia and the public sector to meet and share their experience. Secondly, they learn about the latests developments in the field of artificial intelligence (AI). For many people, AI is very distant and vague. They might have heard or read something about it, but they have no idea how they, in particular, might make use of it. Therefore, such events allow people to better understand how software and hardware work together."

Have a look at the full image gallery of AI & HPC ACADEMY 2020

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IT4INNOVATIONS HOSTED AND PARTICIPATED IN EVENTS

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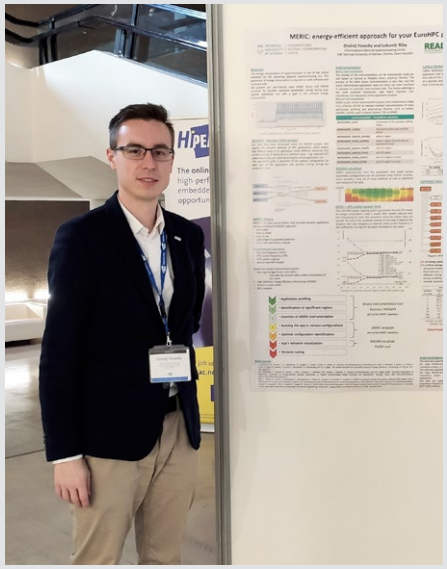
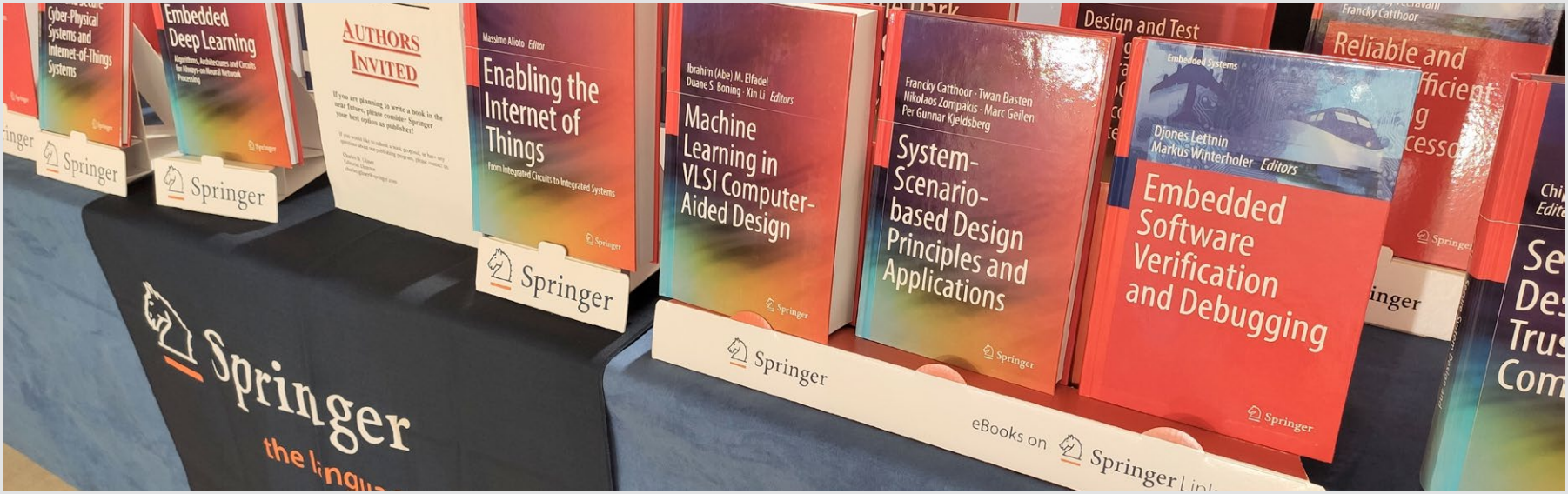
HIPEAC 2020 CONFERENCE, ITALY

At the end of January our colleagues presented their research results at the HiPEAC 2020 conference held in Bologna, Italy. In the poster section the LEXIS project and the MERIC library were presented. For sale at the Springer booth a book entitled System-Scenario-based Design Principles and Applications, featuring a chapter entitled Run-Time Exploitation of Application Dynamism for Energy-Efficient Exascale Computing co -authored by Lubomír Říha, Ondřej Vysocký, and Jan Zapletal. Part of the conference also included the Heterogeneous and Low-Power Data Center technologies HeLP-DC workshop jointly organized by the LEXIS, Evolve, Deep Health, and Cybele projects.





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VISIT OF THE MARSHAL OF THE SILESIAN VOIVODESHIP

At the beginning of February, IT4Innovations hosted Jakub Chelstowski, the Marshall of the Silesian Voivodeship, and other guests including Ivo Vondrák, the Governor of the Moravian-Silesian Region. The purpose of this meeting was to address the potential for cooperation in areas such as ICT, the energy industry, and innovations, all of which was presented by representatives of IT4Innovations, the MSIC, and the Energy and Environmental Technology Centre.

For image gallery from the visit, see

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ŠKOMAM 2020

At the end of January, more then 100 students of the School of Mathematical Modelling (Škomam), organized by the Department of Applied Mathematics at the Faculty of Electrical Engineering and Computer Science at VSB – TUO, visited our centre to participate in lectures as well as take our data room guided tour.

For more, see

DIGITAL TRANSFORMATION 2020

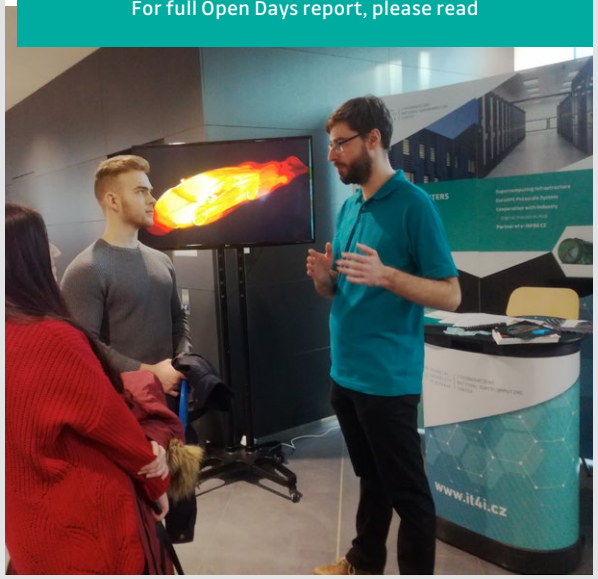
On Wednesday 4th March, IT4Innovations' atrium served as a presentation venue for the CzechInno association, which organized Digital transformation 2020 here. This event also hosted our colleague Tomáš Karásek, who presented our activities in the field of cooperation with industry. This event was concluded with a guided tour around the IT4Innovations infrastructure.

For more about the event, see

WE PARTICIPATED AT THE VSB – TUO OPEN DAYS EVENT

At the VSB – TUO Open Days we shared a booth with the Department of Applied Mathematics where we presented IT4Innovations' activities to young people interested in studies at VSB – TUO.

For full Open Days report, please read



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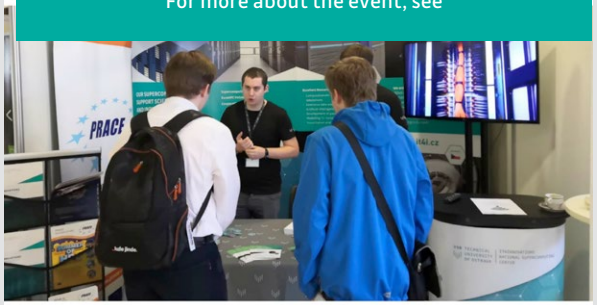
CAREER JOB FAIR KARIÉRA+

No single annually held Career job fair like the 13th edition of kariéra+, organised at the Aula of VSB – Technical University of Ostrava, could do without our presence. In the competition of nearly 100 companies, we held up well at our booth, where we presented our activity and career opportunities at IT4Innovations to interested potential candidates. This year's job fair was visited by more than 2000 people interested in new job opportunities, many of which dropped in on our booth.

For more about the event, see



SCIENCE AT THE MORAVIAN-SILESIAN SCIENTIFIC LIBRARY

By presenting a lecture entitled All you wanted to know about supercomputers but did not know who to ask, Ondřej Vysocký from the Advanced Data Analysis and Simulations Laboratory opened a series of lectures on Science at the Moravian-Silesian Scientific Library on 4th March. The lecture was held at the Moravian-Silesian Library of the City of Ostrava.

INFORMATION NIGHT OF THE FACULTY OF INFORMATION TECHNOLOGY

Information Night at the Faculty of Information Technology of the CUT in Prague, held on Monday 9th March, featured Branislav Jansík, the IT4Innovations Supercomputing Services Director, who presented his lecture entitled IT4Innovations National Supercomputing Center: e-infrastructure for high-performance computing.

For more about the event, see

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