NEWSLETTER Q4/2020

VSB TECHNICAL UNIVERSITY OF OSTRAVA

IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

IN BRIEF

VÍT VONDRÁK AMONG THE TOP IT PERSONALITIES OF THE YEAR 2020

Every year, the Computerworld magazine announces the TOP IT Personalities of the Year poll. As always, it is a mix of innovators, start-up founders, and experienced people who have been in the IT field for a long time. The IT4Innovations Managing Director, Vít Vondrák, has also become one of the top 30 IT personalities of the year 2020.

Profile of Vít Vondrák

THE UNIVERSITY OF OSTRAVA AS PART OF THE DOCTORAL SCHOOL

The Doctoral School for Education in Mathematical Methods and Tools in HPC (MathInHPC) was established by the Faculty of Mathematics and Physics of Charles University in Prague, the Institute of Mathematics of the Czech Academy of Sciences, the Faculty of Electrical Engineering and Computer Science of VSB – Technical University of Ostrava, and IT4Innovations in 2019. The University of Ostrava's Faculty of Sciences has also become a new partner with the Biophysics and the Physics of Nanostructures PhD study programs.

www.mathinhpc.cz

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IN BRIEF

APPLY FOR PRACE COURSES ANYWHERE IN EUROPE

Although the current situation is not favourable at all for organizing conventional courses, there are still opportunities to participate in many online courses. Just choose one or more from a wide range of PRACE courses anywhere in Europe. Courses designed for academics are completely free of charge.

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LEXIS PROJECT PUBLISHING ITS FIRST NEWSLETTER

For all fans of HPC, cloud, and big data, the LEXIS project has published its first newsletter, which provides more information about the project, its planned activities, and summarizes the project's achievements over the past few months.

lexis-project.eu/web

HPCSE PROCEEDINGS AVAILABLE

The HPCSE 2019 Conference Proceedings published by Springer is now available for downloading.

For downloads, see HERE.

SCTRAIN PROJECT TO RAISE AWARENESS REGARDING HPC

IT4Innovations is part of the SCtrain project, the mission of which is to use a systematic approach to fill gaps in current university courses and raise awareness of HPC for future experts in science, technology, engineering, and mathematics. In addition to IT4Innovations, the Faculty of Mechanical Engineering of the University of Ljubljana, the Austrian Vienna Scientific Cluster supercomputer centre, and the Italian CINECA supercomputing centre are collaborating on the project.

SCtrain | SUPERCOMPUTING KNOWLEDGE PARTNERSHIP

sctrain.eu

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MEET KAROLINA

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The new most powerful Czech supercomputer is going to be called Karolina

In the final quarter of last year, there was a competition to name the most powerful supercomputer in the Czech Republic, which will be installed in IT4Innovations this year. From more than 5,000 proposals sent by over 2,000 people, the name KAROLINA was selected by the jury.

The public competition to name the new supercomputer was launched in October last year. In total, 5,114 proposals were received in two months, with over 2,000 people voting. From the proposals received, 3 winners were selected, and they will receive valuable prizes from Hewlett Packard Enterprise, which will deliver the Karolina supercomputer. Among the most frequently nominated names were those of mythical or fictional persons (Golem, Bivoj, Cimrman, Perun, and Sheldon), well-known scientists and thinkers (Amos, Albert), and places and former mines in the Moravian-Silesian Region (Ema, Landek, Odra, Karolina). The 10-member jury thus faced the daunting task of selecting a name that would be original, concise, one-word, well-spoken in both Czech and English, and composed of four to eight letters that would not contain special characters or diacritics.

"In the past, names relating to the Moravian-Silesian Region have always been chosen, and I am personally pleased that the tradition in Karolina's case has been observed," says Vít Vondrák, IT4Innovations Managing Director. *"I believe that the Karolina supercomputer, which has the best prospects to rank among the 50 most powerful supercomputers in the world, will build a great reputation through being accessible not only to Czech but also to European scientific and industrial users,"* adds Vondrák.

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

KAROLINA SUPERCOMPUTER

The Karolina supercomputer will achieve a theoretical peak performance of 15.2 PFlop/s. The installation of this unique computing system is already underway to make it fully operational in the first half of 2021. Its service to science, industry, and society is expected to run to the year 2025.

For more information and images from its installation, see HERE

WHY KAROLINA?

It has always been a tradition that the names for the supercomputers operated at IT4Innovations National Supercomputing Center in Ostrava are chosen by the public. This was the case with Anselm, Salomon, and Barbora. The name Karolina refers to another mine in the Ostrava-Karviná coal basin, which was named by Salomon Rothschild after his wife, Caroline. Besides, all the names referred to the strong mining tradition and industrial history of the Moravian-Silesian Region. Indeed, the Karolina coking plant located at the very centre of Ostrava until the 1980s is still vividly remembered and inextricably linked to Ostrava by the people of Ostrava.

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PROJECT DATA STORAGE

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New data storage for IT4Innovations users

In January, IT4Innovations finished installing a new user data storage, which for the first time will not be part of the computing cluster as it was in the case of Anselm, Salomon, and Barbora. The procurement of an independent data storage was undertaken by IT4Innovations, taking into account the different lifespan and duration of support for individual technologies, with data storages typically outperforming computing technologies in terms of their lifespan.

User data on computing clusters has a different lifespan with respect to its purpose, which is why clusters are often procured with different data storages. Typically, less powerful and low-capacity solutions (so-called HOME storage) are procured for the single purpose of user account existence, while high-performance and medium-sized solutions (so-called SCRATCH storage) are procured for the actual execution of calculations, and finally for the long-term storage of data beyond the life cycle of individual annual projects, as large as possible but still reasonably efficient solutions are procured. And this is precisely the case with the new data storage professionally referred to as the PROJECT storage.

"IT4Innovations projects often combine the use of multiple computing technologies, so it makes sense to acquire new storage outside the framework of a particular cluster, and in turn to ensure its full availability in the same way across all existing and future systems. While this has the disadvantage of not being natively integrated into a high-speed computing network, (unlike SCRATCH), it does bring the benefit of that universal and unified application for users," says Filip Staněk, Senior HPC Architect at IT4Innovations.

The data storage itself is modularly designed to allow for an uninterruptible extension of capacity in the future, thereby ensuring users uninterrupted use. From a technical point of view, a key feature is the high availability provided by redundant elements from the drives themselves to their controllers, servers, and clusters, the use of RAID technologies, and the cluster solution to the operation of data-providing servers.

Along with the new storage, users will be offered a sufficiently dimensioned space for their data both in terms of capacity and performance. Despite future servicing and upgrading of storage and computing systems, which will improve both data security and accessibility, user data will remain accessible. The data will be available to users with unified access from all the computational resources they use, and with the ability to replicate the critical data over individual blocks. Overall, there will thus be an increase in the quality and ease of working with the data of individual projects.

The storage procurement was performed as part of the IT4Innovations National Supercomputing Centre – path to exascale project. The DATERA company, who specializes in data storage design and implementation, and also supply one of the data storages for CESNET (a member of e-INFRA CZ together with IT4Innovations) was selected as the solution supplier through an open tender.

TECHNICAL SPECIFICATIONS:

- The total storage capacity is 15 PB with a total throughput of 39 GB/s and an output of 57,000 IO operations per second, and is organised into three fully independent blocks, taking into account the mentioned high availability and simple possibility of data replication.
- IBM SpectrumScale to allow advanced features such as snapshots to ensure quick recovery of data that are accidentally deleted by users or that are damaged due to technical failure.
- NFS protocol to ensure wide availability across all IT4Innovations computing units.
- High-speed transmissions using the GridFTP protocol.
- The unit is connected to the WAN network via a pair of powerful Cisco network switches with an aggregated switching capacity of 14.4 Tb/s.

This project was supported by the European Regional Development Fund (ERDF) as part of the IT4Innovations National Supercomputing Centre - path to exascale project (CZ.02.1.01/0.0/0.0/16_01 3/0001791) implemented under the OP RDE.

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VISUALIZATION AND VIRTUAL REALITY LAB

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IT4Innovations has launched the Visualization and Virtual Reality Lab

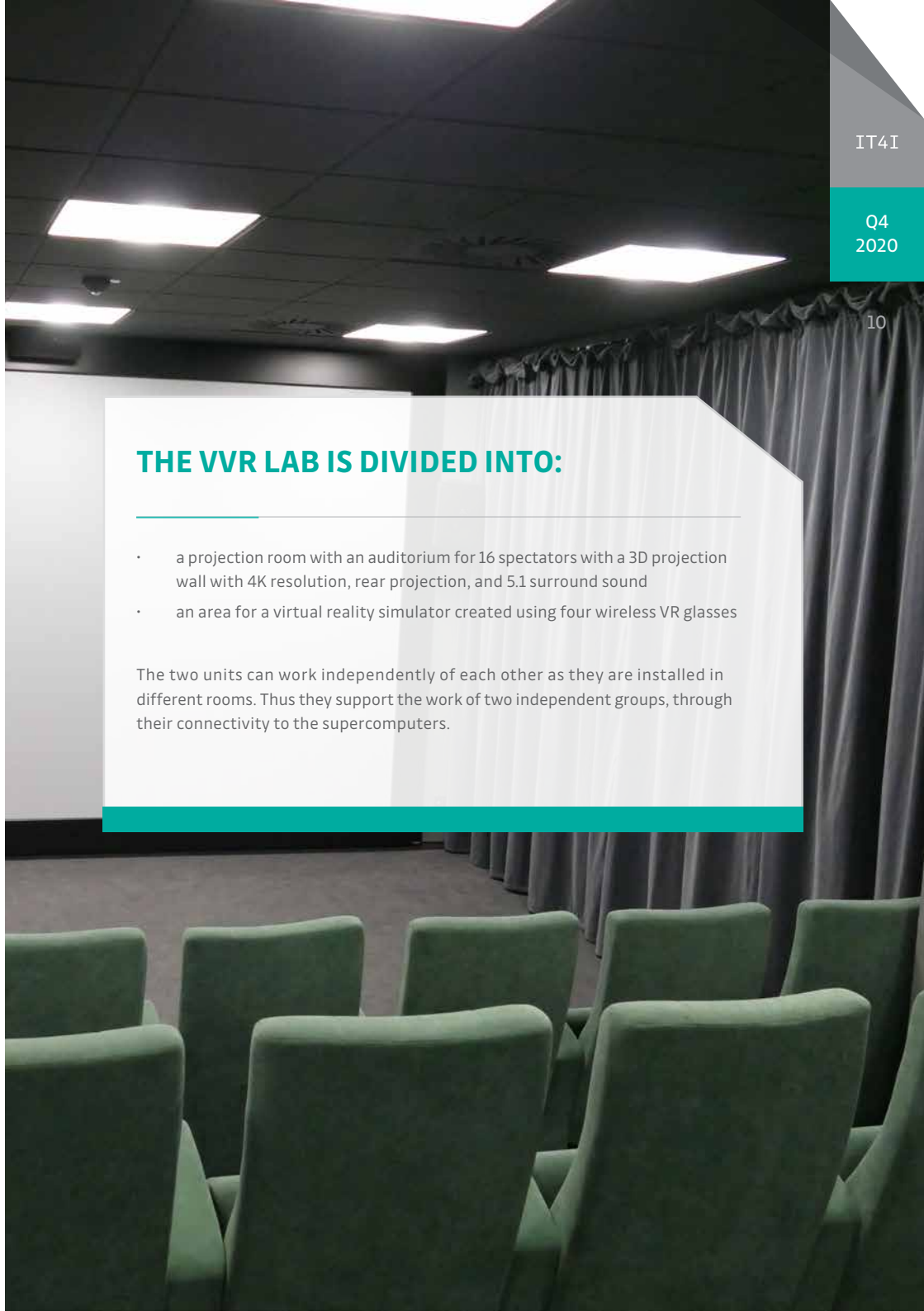
At the end of last year, IT4Innovations launched the Visualization and Virtual Reality Lab (VVR Lab), which will support the supercomputing infrastructure, and is to be used to visualize 3D content using the latest available technology in large-scale 3D projection and virtual reality devices. Among other roles, the lab will support in-house research carried out at IT4Innovations and at VSB - Technical University of Ostrava.

In particular, the lab will find its use in visualizing large-scale scientific calculations, such as projects in engineering, nanotechnology, material design, and many others. Moreover, it will also be used in cooperation with industry partners, in particular to visualize the results of joint research, verify prototypes, and present products. Last but not least, it can also help with educational activities such as teaching anatomy in 3D, demonstrating product manufacturing processes, and as a general simulation training device.

Lab equipment description

The solid 3D projection wall in the projection room is illuminated by Barco's top-of-the-line 3D laser cinema projector with high 4K resolution. The projector is installed behind the wall so that users examining the results presented can move in the immediate proximity of the projection screen without casting a shadow on it, as they would with a forward projection. The image projected by the projector is generated by a computing station directly installed in the projection room or by a computing cluster in the IT4Innovations data room. The newly built 100 Gb/s Ethernet line between the data room and the VVR Lab is designed to transmit data and images directly from the IT4Innovations supercomputers. The image generating stations for individual VR glasses are also connected to this line.

The VR simulator area is designed to accommodate the cooperation of up to 4 people in virtual reality. It is based on a trio of wireless HTC Vive Pro glasses with 2K resolution for each eye. With these glasses, the image is transmitted from the rendering station by wireless technology, and the user's movement is not restricted by cables. Another important feature is the VR XTAL glasses from the Czech VRgineers company with high 4K resolution for each eye. Even in the case of these glasses, there is no restriction on cable movement, as the image is generated by a special VR backpack (i.e., a computer on the back). The rendering stations for VR glasses are located directly in the lab and are also connected by a fast 100 Gb/s Ethernet line to the data room, so that the image can be directly generated on the IT4Innovations supercomputers.



THE VVR LAB IS DIVIDED INTO:

- a projection room with an auditorium for 16 spectators with a 3D projection wall with 4K resolution, rear projection, and 5.1 surround sound
- an area for a virtual reality simulator created using four wireless VR glasses

The two units can work independently of each other as they are installed in different rooms. Thus they support the work of two independent groups, through their connectivity to the supercomputers.

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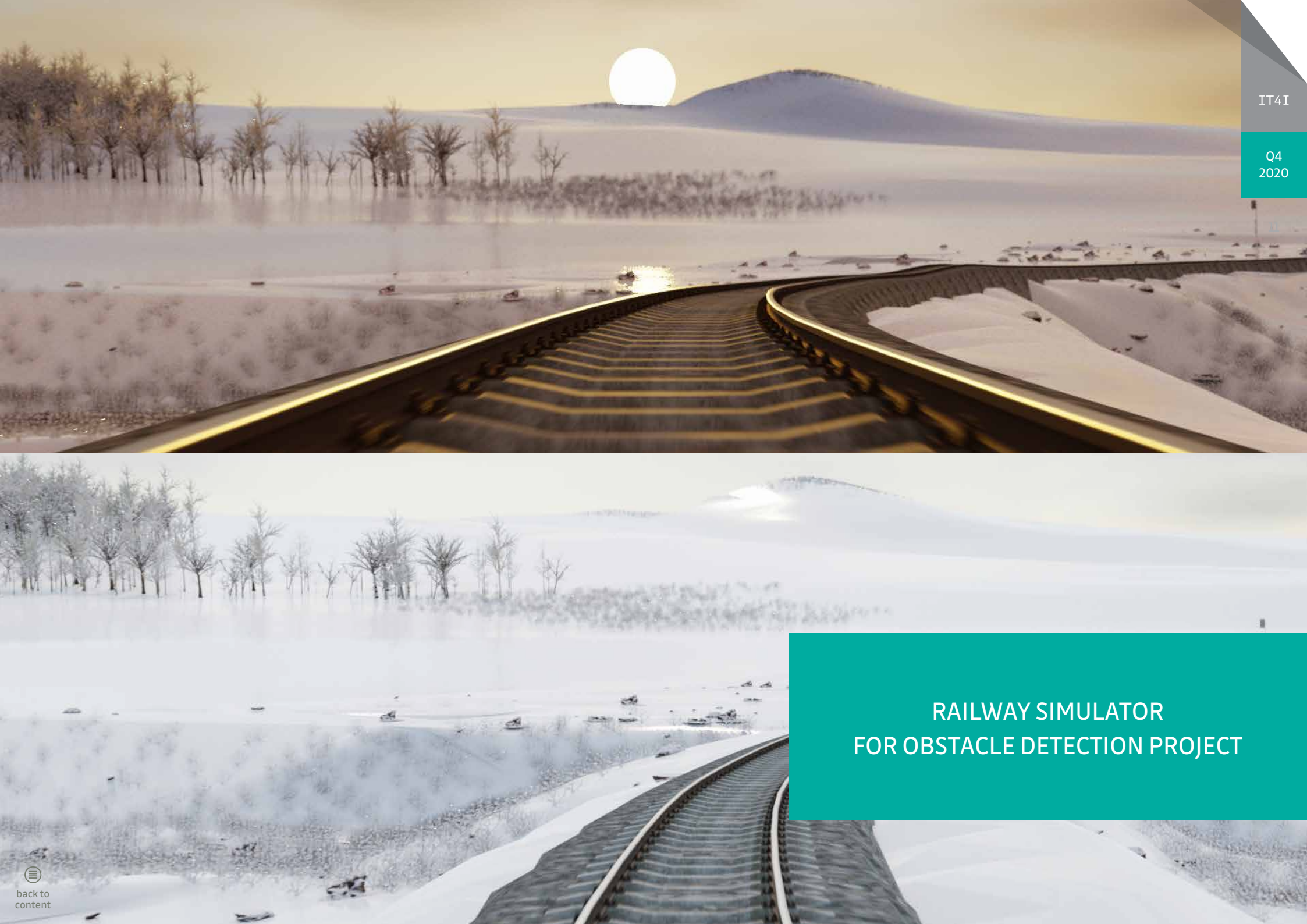

RAILWAY SIMULATOR FOR OBSTACLE DETECTION PROJECT

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The first phase of the Railway simulator for obstacle detection project has been completed

In January last year, 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' was launched at IT4Innovations in cooperation with the IXPERTA s.r.o. company. 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 will be used. As a key support for development of the detection system, the project includes the development of a software simulator for virtualization of railway conditions as well as implementation of test rides in a laboratory environment.

In such an environment, it will not only be possible to create crisis situations, which can analogously arise on a real railway track, but also to simulate various weather phenomena such as rain, snow, and fog, which can influence the generated output data. The simulator solution will include specification of particular critical scenarios that may occur, and selection of important virtual environment parameters that can be influenced, in particular, to define the complexity of the simulator while ensuring the required variability and credibility of data necessary to train the detection algorithm.

The project, in which IT4Innovations is responsible for creating a 3D virtual simulator environment and generating enough quality data to train a detection algorithm, is currently in its first phase. IXPERTA have designed the construction for the sensors, fitted the test railway vehicle with these sensors, and started data collection. A visual camera, a thermal camera, a laser sensor, and a train positioning sensor were used with the aim of enabling detection of objects at all times on the track. Analogous sensors will also be used when creating a software simulator at IT4Innovations.

Unlike in the case of automotive transport, there is currently no available, generic software on the market that can do virtual replication of inputs for a learning detection system on a real railway track, including climatic and other limiting conditions. *"In order to create a reliable virtual railway environment, it was necessary to take into account large amounts of data such as terrain elevation, vegetation grids, real train speed profiles, and different types of static or dynamic objects. Due to the computational demands of the data generated, the IT4Innovations infrastructure is used as part of the project,"* says Petr Strakoš, Principal Investigator of the project at IT4Innovations.

In the first phase of the project, a section of the railway track between Třebenice town and Dlažkovice stations was modeled. A 3D scene containing the underlying terrain, vegetation objects, and the track curve used to model the railway tracks (embankment, track, and sleeper objects) has been created. Based on the date and time specified, the particular phase of the day was calculated and the position of the sun and the appearance of the sky set. Static and dynamic objects, which are then placed in the scene, have been created for the track. A prototype train object with a camera and other features necessary for simulating sensors has been incorporated into the created environment. Based on the given events, the movement/animation of the train and other dynamic objects has been calculated. Various climatic conditions and weather phenomena can be simulated in the generated environment. In the first phase of the project, phenomena such as clouds and snow were in the experimental stage.

The current outputs that the simulator is able to generate are images from an RGB camera, a depth map, LIDAR, and a segmentation map with a ground truth classification. The depth map is obtained automatically using the ray tracing method, and can be used in the future as a resource to calculate LIDAR data so far having been obtained in a different way. Ground truth recording is an important output that is necessary to train the obstacle detection algorithm, which will take place in the next phase of the project. At the same time, train location information in GPS coordinates and train orientation information (azimuth, elevation) is also generated in a textual form.

The second phase of the project will continue with the simulator implementation. Emphasis will be placed on achieving a higher degree of lifelike synthetic data visualization by modifying augmentation filters based on neural networks. A railway track between Žďár nad Sázavou and Nedvědice stations will also be modeled with the aim of achieving maximum correspondence between the model and the real section of the railway track. Verification of selected concepts used in the simulator with real behaviour will also play an important role in this phase of the project. This may include, for example, the fidelity of the virtual train movement and a comparison of the similarity of the simulated selected sections with real sections of the railway track, etc.

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C R

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 Program.

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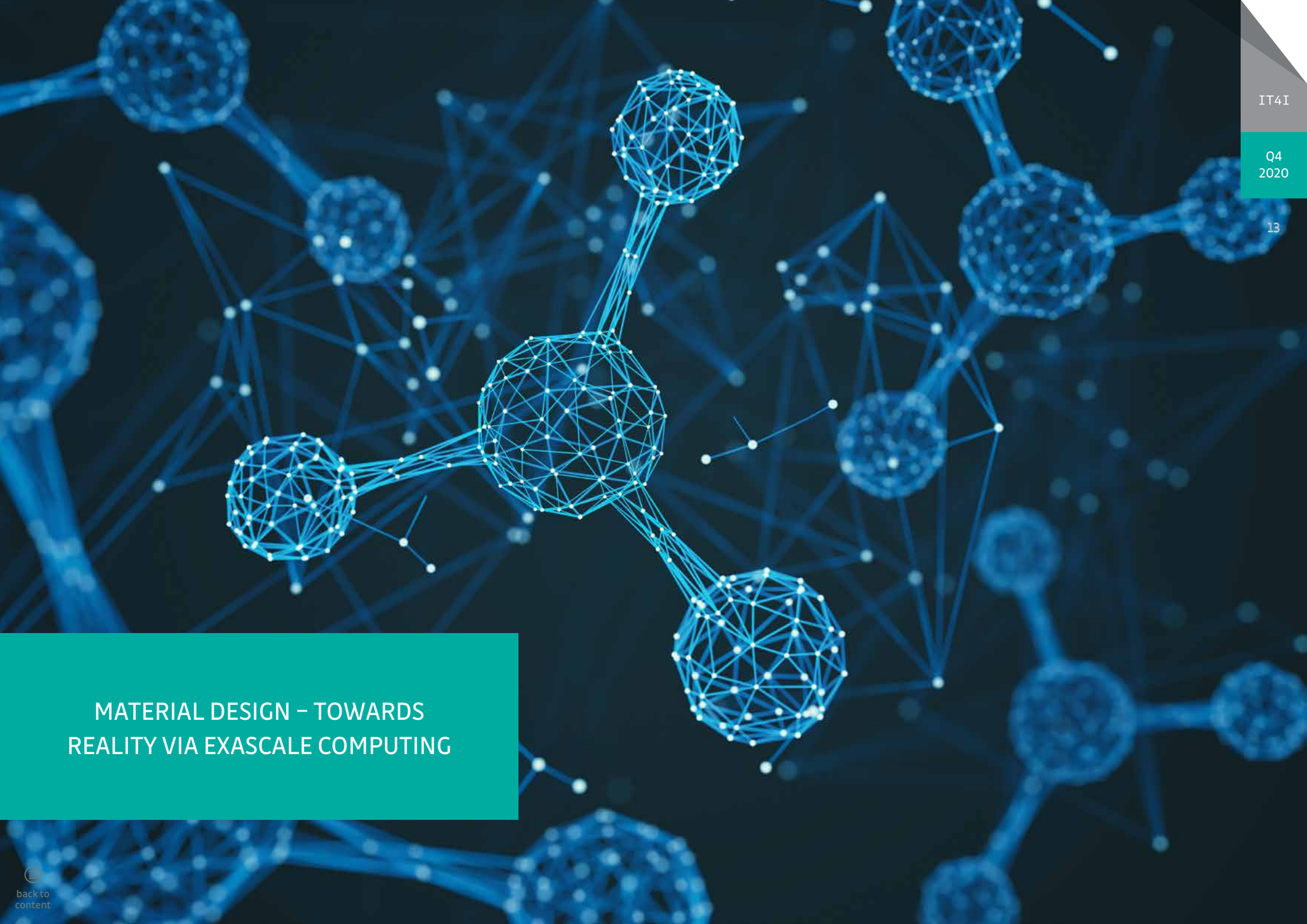

MATERIAL DESIGN – TOWARDS REALITY VIA EXASCALE COMPUTING

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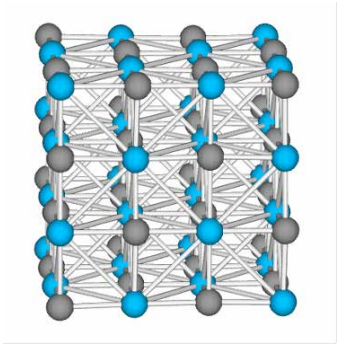
Material design – towards reality via exascale computing

The third IT4Innovations research flagship is focused on performing large multiscale calculations across various lengths and timescales, beginning at quantum-level (ab initio) calculations up to atomistic ones, and simulations of classical molecular calculations as well as micromagnetic simulations that are close to the level of finite element methods. The main research topics are related to phenomena beyond lattice vibrations and magnetism in 3D as well as at heterostructures and 2D materials. Read about the main scientific directions of this research flagship.

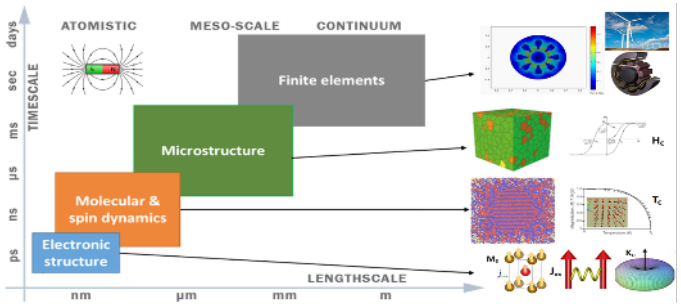
Scientific direction: Lattice and Atomistic Vibrations - 3D and 2D materials

Solids, molecules and atoms vibrate even at T=0K around their equilibrium positions. These collective lattice motions (phonons) are responsible for many interesting phenomena like thermal expansion, superconductivity, etc. Due to the computational power of IT4Innovations HPC, these phenomena can be described at an atomistic scale, and thermal expansion and heat capacity of any materials can be determined directly from quantum-mechanical calculations without any empirical parameter. The research team models IR and Raman absorption spectra and mutual interaction of phonons to understand how heat is transported, and what it affects in matter. These calculations allow the design of novel nuclear fuels, searching for ultra-hard solids similar to diamond, as well as improving the figure of merit of thermoelectric materials. Another specific area of interest of our colleagues within this flagship is the study of phonon-electron and phonon-spin interaction. This allows superconductivity to be modeled. Moreover, for the very first time magnetic materials can be modeled under finite temperatures directly using quantum-mechanical calculations aiming to describe the behaviour of magnetocalorics (cooling with a magnetic field, and understanding ultrafast demagnetization by laser pulse for novel data-storage techniques



Scientific direction: Magnetism studies

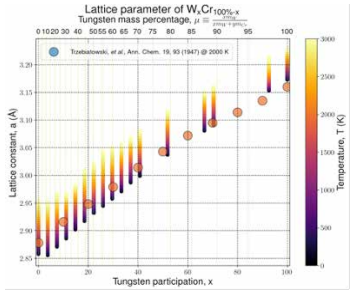
The flagship research team also studies, models, and designs magnetic materials at different spatial and time scales for several technological applications such as magnetic recording, spintronics, electric motors, electric generators, magnetic actuators, biomedicine (magnetic hyperthermia), magnetic refrigeration, etc. They apply

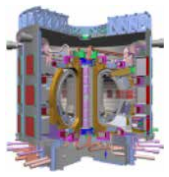


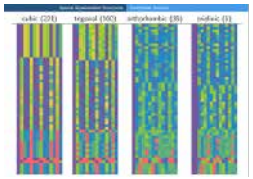
and combine modeling techniques to describe and understand magnetic materials accurately. Some of these approaches use Density Functional Theory (DFT) to calculate magnetic intrinsic properties at the microscopic scale and novel structures predicted by evolutionary algorithms, atomistic spin dynamics (to take into account finite-temperature effects), molecular dynamics (to study grain boundary phenomena and crystal phase stability), micromagnetics (to calculate magnetic domains, microstructure effects, and hysteresis loops at the macroscopic scale) and multiphysics finite-element models (to simulate magnet performance at operating conditions).

Scientific direction: Transition Metal and High Entropy Alloys Modeling

Within the research of clean energy technologies, new alloys for novel thermonuclear fusion reactors, such as ITER (International Thermonuclear Experimental Reactor) are designed using realistic, quantum-mechanical models for real simulation of First Wall alloys in reactor vessels, which are exposed to the heat of hydrogen plasma with a temperature of cca 200,000,000 °C, protected only by an external magnetic field (5T) keeping the plasma confined. Combining Quantum Mechanics, Statistical Physics, and High-Performance Computing, the used methods thus create a kind of a synergic modeling engine. Recently, surprising properties were obtained for 5-components equiatomic alloys stabilized by the entropy term at high temperatures with properties much different to those single







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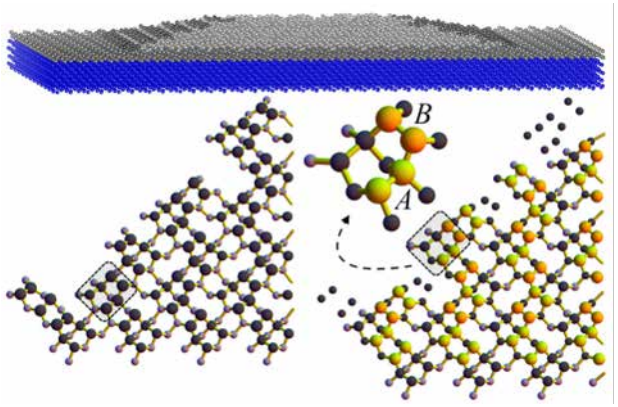
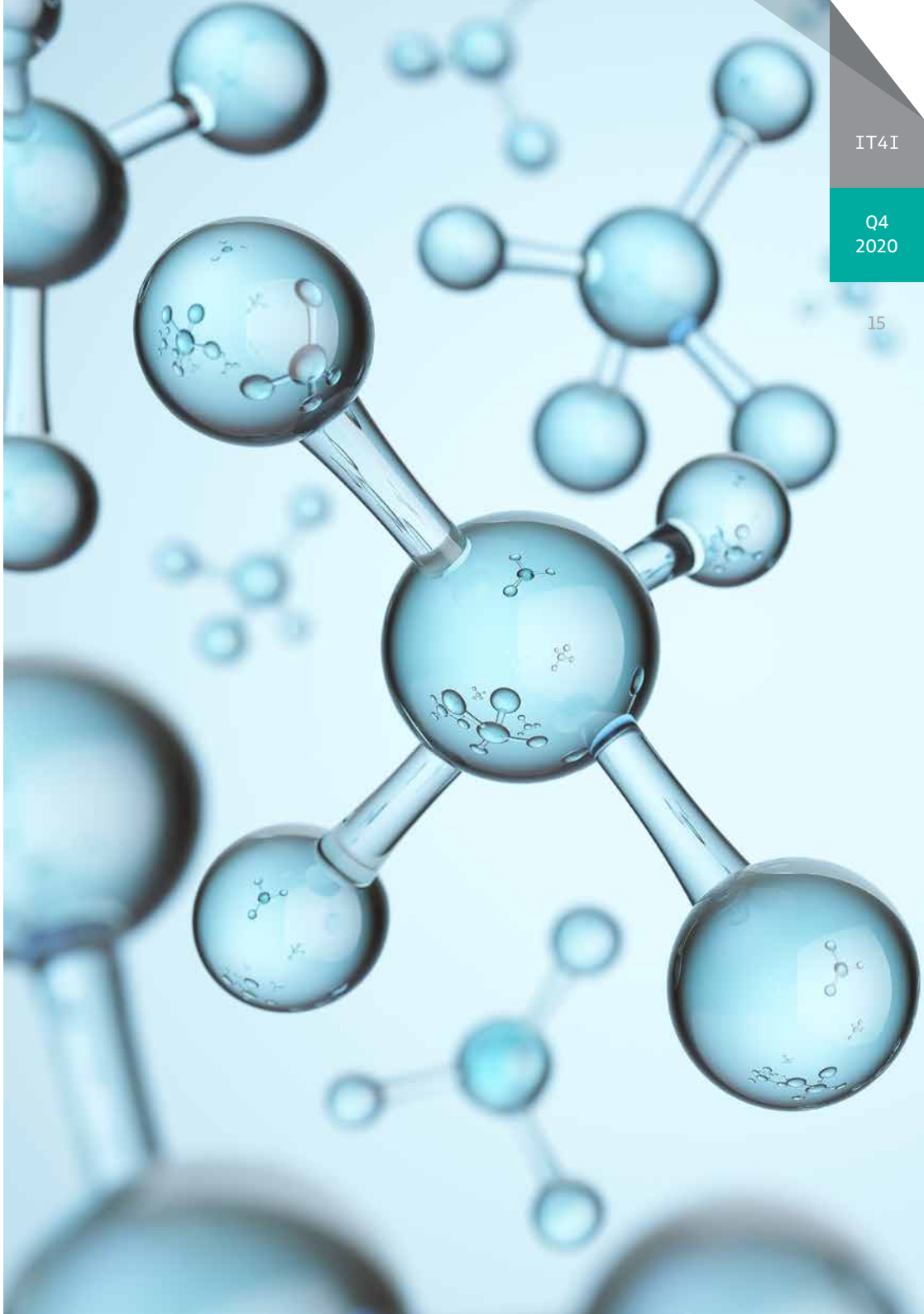


element constituents. A new category of so called high (HEA), middle, and low entropy alloys has been instigated. Despite energies mostly being focused on the mechanical properties, magnetic behaviour cannot be omitted, as it is able to influence the phase stability and mechanical properties. The very first HEA is composed of Cr-Mn-Fe-Co-Ni being surprisingly paramagnetic at RT. Thus the objective is to determine the effect of the composition and substitutions on the magnetic character here.

Scientific direction: Large-scale Atomistic Simulations

Design and prediction of physical properties for realistic materials requires accurate calculation of large systems of atoms. Electronic structure calculations based, for example, on DFT became, in fact, the main computing method in materials science. However, standard DFT calculations deal with relatively small system sizes of a few hundred atoms, both for the purpose of computing time and memory requirements as computational intensity increases with the square and cube of the number of atoms. For more realistic systems with dislocations, interfaces, grain boundaries, random and diluted alloys, nano-particles, and biomolecules, however, it is necessary to perform simulations of an order of several thousand to several million atoms. The CONQUEST code, utilizing the density matrix approach with a local basis, is a very efficient parallel method that provides a linear scaling solution. Such calculations are capable of an accurate description of the growth processes of nano-sized systems such as nano-particles, quantum dots, and nano-wires.

Another large-scale atomistic modeling method is the molecular dynamics approach based on interatomic potentials. For many applications, it allows physical properties behaviour to be determined under a given temperature (diffusion, melting temperature, coexistence of different phases). In such cases, DFT calculations would again be prohibitively expensive, or even unfeasible due to running long simulations in the order of nanoseconds, even when using the CONQUEST code. Within the research, machine and deep learning methods are applied to design accurate interatomic potentials from DFT calculations.



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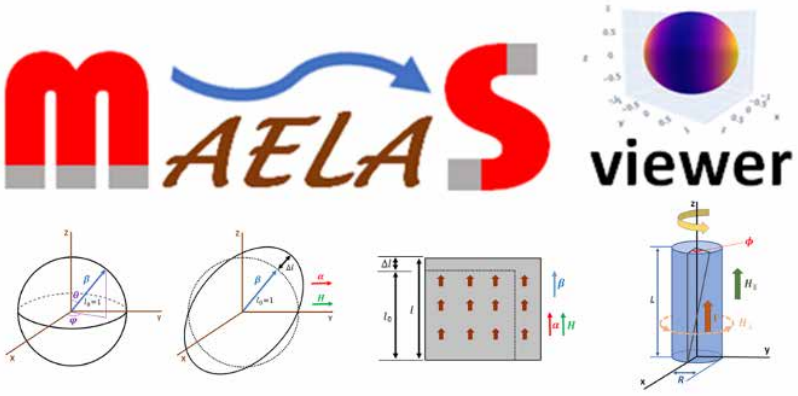
SCIENTIFIC DIRECTION: CODE DEVELOPMENT

The flagship researchers develop several codes written in the Fortran, Python, and Matlab/Octave programming languages. Below there is a selection of those that have already been published and made publicly available.

- PNADIS: This code is an automatic analyser of the Peierls-Nabarro stress and dislocation cores developed in MATLAB. This code calculates the dislocation core structure, Peierls stress, the pressure field around the dislocation core, and the solid solution strengthening of a crystal based on the Peierls-Nabarro model and other models derived therefrom.

- MAELASviewer: An online application for visualization and analysis of magnetostriction via a user-friendly interactive graphical interface.



MATERIAL DESIGN FOR INDUSTRY: COOPERATION WITH CONTINENTAL CZECH REPUBLIC

To design many technological applications, it is necessary to understand the physical and chemical processes occurring at the macroscopic level. Many miniature electronic devices are embedded into protective materials (silica, polymers, etc.), which may degrade in certain environments (gasoeus, liquid) and under certain conditions (high/low temperature and/or pressure). Such processes can be simulated for realistic models (large systems of 104–106 atoms) using classical Molecular Dynamics (MD) with reactive force field (ReaxFF). This interaction potential is a trade-off between accuracy, provided by DFT calculations, and the system size and the length of the temporal evolution of the system. These simulations allow various interfaces between materials and the environment (gas-solid and/or liquid-solid interface), structural stability under various pressure and temperature conditions, and the diffusion of various molecules into the material and its effects on its properties to be modeled. This knowledge may provide prompt technological solutions for industry (design of new materials, protective layers, and optimal operation conditions) similarly to those designed for the Continental Czech Republic company in 2019.

PRINCIPAL INVESTIGATOR

- Dominik Legut

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EVALUATION OF THE 20TH OPEN ACCESS GRANT COMPETITION

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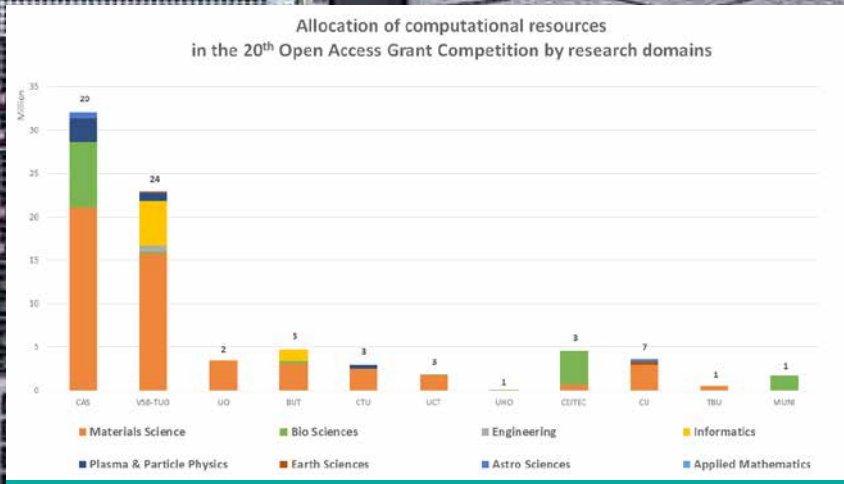
Evaluation of the 20th Open Access Grant Competition

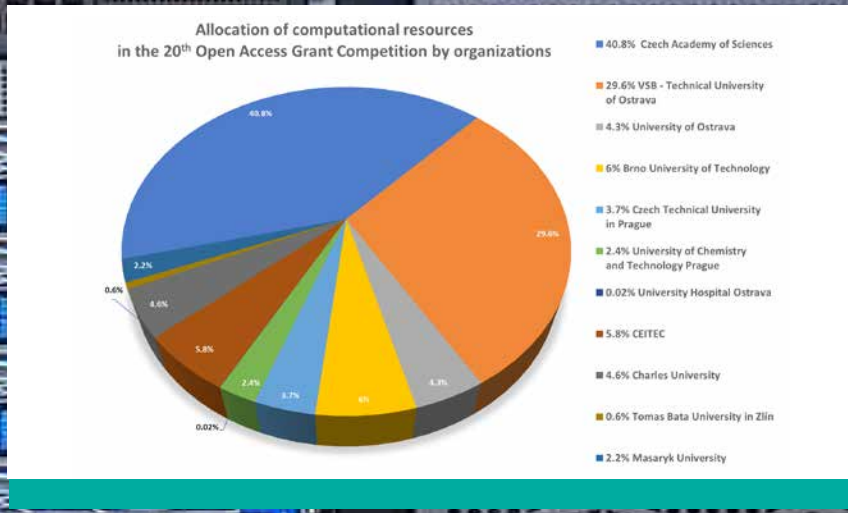
In the 20th Open Access Grant Competition (OAGC), interested candidates for computational resources applied for nearly 148 million core hours. The requested resources exceeded the dedicated capacity of 78.6 million core hours by 88 %. With respect to the high demand for computational resources in relation to the amount offered, the Allocation Committee decided to decrease the initial allocation for each individual project. The reductions proportionately affected all projects. For this OAGC, the Allocation Committee therefore redistributed more than 78.6 million core hours across 70 successful projects with 25 of them being multi-year ones. The Committee has also decided on allocations for the next period of multi-year projects submitted in the previous Open Access Grant Competitions.

Over 32 million core hours have been allocated to researchers from the Czech Academy of Sciences institutes for 20 projects, which is more than 40% of the total computational resources. Across 24 projects, the researchers of VSB – Technical University of Ostrava received more than 23 million core hours, which is about 30% of the total reallocated computational resources, and the third institution with the highest amount of core hours was Brno University of Technology. Its researchers received nearly 4.7 million core hours, amounting to 6% of the total computational resources, for five projects.

Allocation of computational resources in the 20th Open Access Grant Competition by research domains and organizations

An allocation of more than 1 million core hours was awarded to 24 projects of researchers from the Czech Academy of Sciences, VSB – Technical University of Ostrava, Charles University in Prague, the University of Chemistry and Technology in Prague, Brno University of Technology, Masaryk University in Brno, the Czech Technical University in Prague, CEITEC research centre, and the University of Ostrava. The first three most successful projects were awarded a total amount of more than 16.6 million core hours. More than 6 million core hours out of the total amount were awarded to Mojmír Šob from the Czech Academy of Sciences for his project entitled 'The entropy-driven segregation of impurities at grain boundaries'. More than 5.3 million core hours were awarded to Pavel Hobza from the Czech Academy of Sciences for his project entitled 'In silico drug design'. Finally, the third highest allocation was awarded to Dominik Legut from IT4Innovations for his project entitled 'Multiscale design of novel Rare Earth free permanent magnets'.





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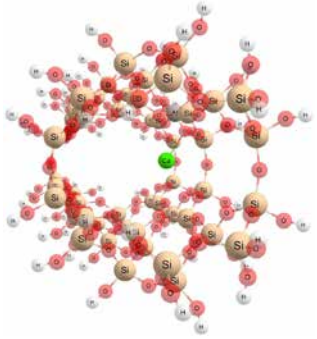
LET US INTRODUCE SOME OF THE SELECTED PROJECTS AWARDED THE COMPUTATIONAL RESOURCES OF IT4INNOVATIONS IN THE 20TH OPEN ACCESS GRANT COMPETITION:

Doc. Václav Čuba
Czech Technical University in Prague

MOLECULAR MODELING AND DYNAMICS STUDY OF MATERIALS FOR USE IN CONTROLLED RELEASE FERTILIZERS

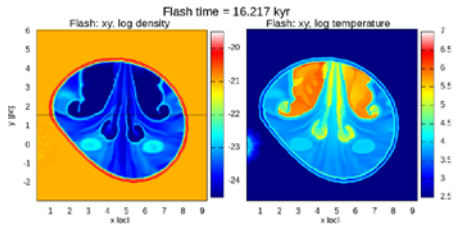
Introduction of NPP (nitrogen, phosphorus, and potassium) and other composite fertilizers made care of soil and plants much easier for farmers. These fertilizers increased yield but caused new and unforeseen ecological problems. To reduce environmental stresses connected mainly to an excess of nitrogen in soil and underground water, new slow and controlled release fertilizers, which copy the curve of plant nutrient uptake with their curve of nutrient release, were developed. This project is focused on finding and studying materials that are useable as a base for slow release fertilizers able to release nutrients in a controlled manner to the environment. Such promising materials seem to be zeolites, the properties of which allow the preparation of a fertilizer containing all essential nutrients, as well as having slow release properties. The binding of molecules of nutrients with zeolitic structures will be studied by molecular modeling methods. From the modeling results, it is possible to predict how the release of nutrients will take place, and what the difference in the strengths of the bonds between each nutrient and the zeolitic structure will be. The aim of the project is to study the possibilities of preparing slow release fertilizers.



Barnabas Barna
Astronomical Institute of the Czech Academy of Sciences

EXPANSION OF SUPERNOVA DRIVEN SHELLS NEAR THE GALACTIC CENTER

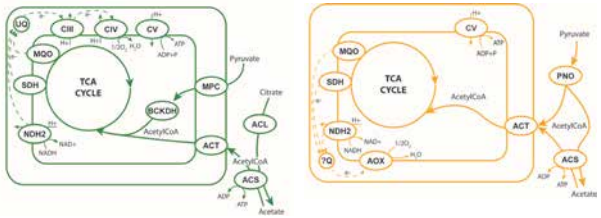
Supernova explosions are some of the most energetic events in the universe. These cataclysmic stellar deaths release chemically enriched material that expands at a high velocity into the surrounding space. The resulting bubble then sweeps around the surrounding interstellar mass, forming an envelope with a mass of several hundred suns. In doing so, it plays an important role in the generation of stars, with expanding bubbles triggering the formation of other stellar generations. Interstellar material can be transported into close proximity to the central supermassive black hole by expanding shells, thus increasing its activity. Whether this scenario is responsible for the manifestation of the supermassive black hole in the Milky Way, however, cannot be confirmed, largely due to the low activity of this nearest supermassive black hole. Simulating the development of shells and the influence of initial and marginal conditions requires numerical methods. Barnabas Barna and his collaborators plan to use the awarded core hours for hydrodynamic simulations with FLASH code in 3D. The objective is to explore the interaction of an interstellar environment with an expanding shell. The results will be matched with current observations: e.g., the current distribution of supernova remnants will be compared to powerful X-ray flashes from the past.



Dr Martin Kolísko
Institute of Parasitology of the Czech Academy of Sciences

GENOMIC INVESTIGATION OF ORGANELLAR EVOLUTION AND ENVIRONMENTAL ADAPTATION IN APICOMPLEXAN PARASITES

Apicomplexa are a group of intracellular parasites of animals and include, for example, agents of the serious human disease, malaria. Although much is known about the genetic makeup and organellar composition of core apicomplexan parasites, gregarines have been largely ignored despite being projected as one of the most species rich groups of eukaryotes. The project aims to characterize representative gregarine lineages from terrestrial and freshwater hosts. Gregarines cannot be cultured, so a method based on sequencing transcriptomes and genomes of individual cells will be used. The obtained data will be used only for phylogenomic analysis in combination with the recently published data on gregarines from marine hosts. This analysis will clarify the evolutionary position of gregarines in the Apicomplexa group, which has recently been challenged by contradictory results from two recently published studies. Robust phylogeny will then allow investigation of both the reductive evolution of organelles across the Apicomplexa group, and also genetic adaptation to different hosts, host environments, and intracellular parasitism occurring in other members of this Apicomplexa group.



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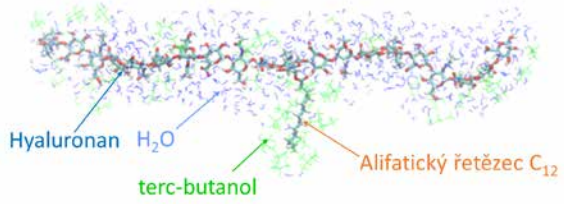
Dr Marek Ingr
Tomas Bata University in Zlín

SUBSTITUTED HYALURONAN MOLECULES IN AQUEOUS AND MIXED SOLVENTS

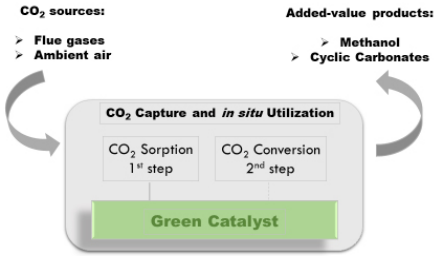
Hyaluronic acid (Hyaluronan, HA) is a key component of the extracellular matrix of skin and connective tissues. It finds wide applications in cosmetics and pharmacology as a compound supporting tissue regeneration and wound healing. As a biocompatible material, it is also used as a base for drug-delivery systems and tissue repair. Although HA is highly hydrophilic, many of its technological applications often require its use in non-aqueous environments. Following previous studies of free HA macromolecules in aqueous solutions and mixtures of water and miscible organic matter, Dr. Marek Ingr and his research team are now looking at the structure of HA molecules substituted by one or more aliphatic chains in the same solvents. The equilibrium behaviour of the molecules is simulated by the molecular dynamics method, from which the molecule's conformation and the mutual position and interaction of its parts, the separation of the mixed solvent around the individual parts of the molecule, the interaction of the parts of the molecules with the molecules in the solution, and in particular the precursors of subsequent substitution reactions, are evaluated. The results of these studies will contribute to optimizing responses leading to the formation of modified HA molecules and the design of materials based on them that can find applications in healthcare, cosmetics, and other fields.



Dr Valeria Butera
CEITEC, Brno University of Technology

DISCOVERY OF NOVEL EFFICIENT CATALYSTS FOR CO_2 CAPTURE AND IN SITU UTILIZATION: DFT INVESTIGATION

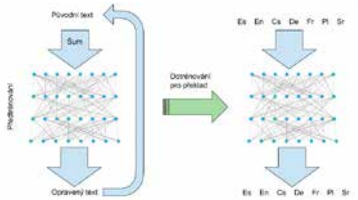
Carbon dioxide (CO_2) is considered the main cause of global warming. Over half of CO_2 emissions are from large industrial point sources, while the remainder of these emissions are from small mobile sources. Reducing its emission below critical levels requires not only political commitment but also novel scientific approaches to capture CO_2 and to enable its conversion from a waste product into value-added products. The key measure to achieve this will be efficient and practicable processes for ambient air and large-scale CO_2 sequestration and utilization. The main focus of this project is the development of innovative technologies aimed at slowing or stemming anthropogenic carbon emissions. The challenge here is the design of new efficient, selective, and "green" homogeneous and heterogeneous catalysts for CO_2 capture and CO_2 conversion. Valeria Butera and her team will first focus on materials that are suitable for CO_2 sequestration and conversion directly from ambient air (direct air capture, DAC). The results of this investigation will pave the way for developing suitable technologies to extract CO_2 from large industrial sources.



Josef Jon
Brno University of Technology

MASSIVELY MULTILINGUAL AND SELF-SUPERVISED NEURAL MACHINE TRANSLATION FOR LOW-RESOURCE LANGUAGES

Machine translation of human language has made tremendous progress due to recent improvements in machine learning. Translations generated by neural machine translation (NMT), under specific conditions, are even comparable to human translation. One of these conditions is that for a given language pair, there are large numbers of parallel, human-translated texts available to train the model. This is true only for a very limited number of language pairs. Improving NMT quality in other languages is based on pre-trained models of neural networks to represent the language. These make it possible to take advantage of large volumes of texts found on the internet, but to which noise is artificially added, with some words being dropped or replaced. The challenge is to reconstruct the original text. By training on this task, the model actually learns to represent and understand language incidentally because these skills are needed to correct the text appropriately. Pre-trained models can be fine-tuned to end tasks using significantly less data than if they were trained from the beginning. It turns out that the more the method of adding noise in the pre-training phase is similar to the end task, the better the result. The aim of Josef Jon, an engineer who has acquired nearly 1.2 million core hours for his project, is to explore variations of noise functions that are similar to translation (e.g., replacing a word or phrase with its translation), and to use the resulting models for translation in language pairs with little training data.



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CZECH HEAD AWARD

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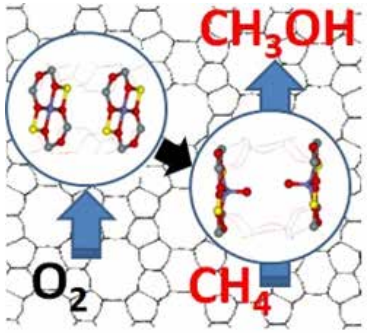
Research with a contribution from IT4Innovations supercomputers won the Czech Head Award

Jiří Dědeček together with Edyta Tabor and Štěpán Sklenák from J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences found a unique way to turn methane into methanol, for which they received the Czech Head Invention Award. Using the IT4Innovations supercomputers in their research, they computationally predicted results, which they eventually confirmed experimentally. They received 32,458,000 core hours of IT4Innovations computational resources for their research over six Open Access Grant Competitions.

In simple terms, zeolite is leaky quartz, and its uniqueness lies in the fact that silicon and oxygen atoms form an interconnected structure of channels and cavities that accommodate smaller molecules. If reaction centres are present in the channels, zeolites become ideal material for use in catalysis.

A team of scientists from the Department of Structure and Dynamics in Catalysis of the J. Heyrovsky Institute of Physical Chemistry has been intensively researching the use of zeolites for catalysing redox reactions in recent years. One of them is the transformation of methane into methanol. Given the low reactivity of methane, this is currently one of the biggest challenges in heterogeneous catalysis, which is drawing immense attention. Methane is the main component of natural gas and is therefore cheap and readily available. Unfortunately, transporting and storing gas is a lot more complicated than in the case of oil. Plus, we can only use it en masse as fuel.

The use of methane in chemical production is still possible only through indirect, and energy, technologically, and economically intensive processes. The final price of the resulting product, e.g., methanol, is then generally prohibitively high. However, methanol can be used widely as a raw material for chemical production, or as an alternative fuel. The direct oxidation of methane into methanol with molecular oxygen is a way to significantly reduce the

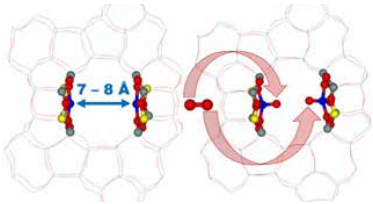


The description of direct oxidation of methane (CH_4) into methanol (CH_3OH) with molecular oxygen (O_2), image: Jaroslav Heyrovský Institute of Physical Chemistry of the CAS

cost of methanol production, bringing us closer to obtaining the technology to produce cheaper fuels, as well as many other industrially usable products.

Until recently, there was no catalyst to convert methane directly into methanol with molecular oxygen efficiently enough. The team of the Department of Structure and Dynamics in Catalysis has created and described the structure and reactivity of new, unique types of reaction centres that can activate oxygen in a previously unknown way - to split it. This can be accomplished by two transition metal cations (e.g., iron) opposite each other, but significantly further apart than in enzymes (at about 7 ten-millionths of a millimetre), at room temperature. This unique system has been successfully used to create methane-to-methanol oxidation systems, as a possible basis for methane technology. The IT4Innovations supercomputers also played a role in the research, helping to predict the results, which were only then experimentally confirmed.

In addition to the ability to split molecular oxygen and oxidize methane into methanol, even at laboratory temperature, the new method exhibits another unique property. Methanol produced by oxidation of methane is also spontaneously released into the gaseous phase at laboratory temperature. This is a very substantial



The description of oxygen split at room temperature, image: Jaroslav Heyrovský Institute of Physical Chemistry of the CAS

advantage over other catalysts capable of selectively oxidising methane with molecular oxygen, where, in addition, it is necessary to use water vapour to release methanol. This then leads to the destruction of active centres and, consequently, to their low level of activity that makes them technically useless in practice.

For more about the research, see HERE.

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DEVELOPMENT OF THE LEXIS PROJECT

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LEXIS brings HPC technologies closer to SMEs, industry and society

This new platform can help industry, society, and especially small and medium-sized enterprises (SMEs) to access and use efficient heterogeneous distributed infrastructures easily and safely without the need for advanced computing knowledge. To lower the entry barriers to the worlds of supercomputing, cloud, and big data, an EU-funded project is testing its platform in the Aeronautics, Earthquake & Tsunami, and Weather & Climate domains.

The increasing quantity of data poses an enormous challenge for organisations seeking to extract knowledge critical for business, operations, and research. The combinations of high-performance computing (HPC), Cloud services, and Big Data technologies are key to meet the needs of large and small organisations alike. However, this has been difficult up to now since the supercomputing centres among the largest in the world have often served solely academic research, for example, in Physics.

"The LEXIS (Large-scale EXecution for Industry & Society) project is building an advanced engineering platform at the confluence of HPC, Cloud services, and Big Data, which uses large-scale geographically-distributed resources from the existing HPC infrastructure, employs Big Data analytics solutions, and augments them with Cloud services," explains Jan Martinovič, the Project Coordinator from IT4Innovations. The platform is driven by the requirements of three initial pilot use cases, and further ones being selected via an open call planned in the second half of the LEXIS project.

The aeronautics pilot mainly focuses on accelerating turbomachinery and rotating -parts simulation workflows by direct code optimization. In addition, advanced hydrodynamics simulation capabilities are now used to predict fluid flow around complex geometries under turbulent motion in the Rotating Parts use-case.

Earthquake and Tsunami simulations and warnings are the focus of the second pilot. The main achievement was a clear formalization of the complex workflows, which run under time-constrained conditions. The computational efficiency of the tsunami simulation code was improved, therefore delivering results of a potential tsunami wave inundation in less than a minute, which enables faster and more accurate emergency warnings.

Last but not least, the Weather and Climate large-scale pilot deals with advanced workflows to predict, for example, flash floods, agricultural yields, forest fires, and air quality, all based on numerical weather forecasts. The models have been packed into ready-to-run containers and virtual machines, and efficient procedures for handling the data and data quality assurance from different sources have been set up. Prototypes of the workflows are implemented and tested on the LEXIS infrastructure, which paves the way for the subsequent assimilation of multiple observational weather data in order to make all our predictions yet more reliable.

To deliver the best user experience, typical user scenarios were collected together with the pilot partners giving invaluable feedback. Based on these, a LEXIS Portal as a one-stop-shop for usage of the platform is being designed. At present, there are prototype views for managing users in the projects, for accessing and listing available datasets, for deployment and running of applications, and for monitoring and billing.

"LEXIS has opted for the security-by-design approach, where security is one of the pillars of the architecture as crucial as compute and data management. A federated, fault-tolerant and modern authentication and authorization framework has been implemented. It provides LEXIS users single-sign-on and role-based authorizations across the entire data and service providers community," points out Marc Levrier from Atos. *"In addition to regular cloud and HPC resources, diverse acceleration technologies (GPU, FPGA, Burst Buffers) can be referred to from the application workflows exposed in the LEXIS portal and allocated by the orchestrator at execution time"* Levrier adds.

The solutions provided by LEXIS will enable improved cooperation between industry and academia. The new platform will ensure that SMEs and industries are able to use the appropriate resources for their applications in a user-friendly manner.

"To improve the quality of the LEXIS platform, we launched an open call in December, in which partners from academia and business will be asked to test their applications on the LEXIS platform and provide feedback. This should also increase the impact of the project and establish a presence in various communities of potential users," adds Martinovič.

Based on the LEXIS pilots, several needs shared by SMEs and industry were identified within a number of different fields:

- dynamic data-aware orchestration of complex workflows;
- data sharing between Cloud and HPC resources and distributed data management with appropriate data backend to the orchestration solutions;
- access to HPC/BigData/Cloud resources for SMEs and industry including novel compute and data acceleration through, e.g., GPUs, FPGAs, and Burst Buffers, and
- easy control of workflows and data through a user-friendly web interface with single sign on to the platform via a federated AAI, and seamless integration of remote visualisation services.

This project received financial support from the European Union Horizon 2020 Research and Innovation Program under Grant Agreement No. 825532.

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ES4G PROJECT

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Energy System for Grids

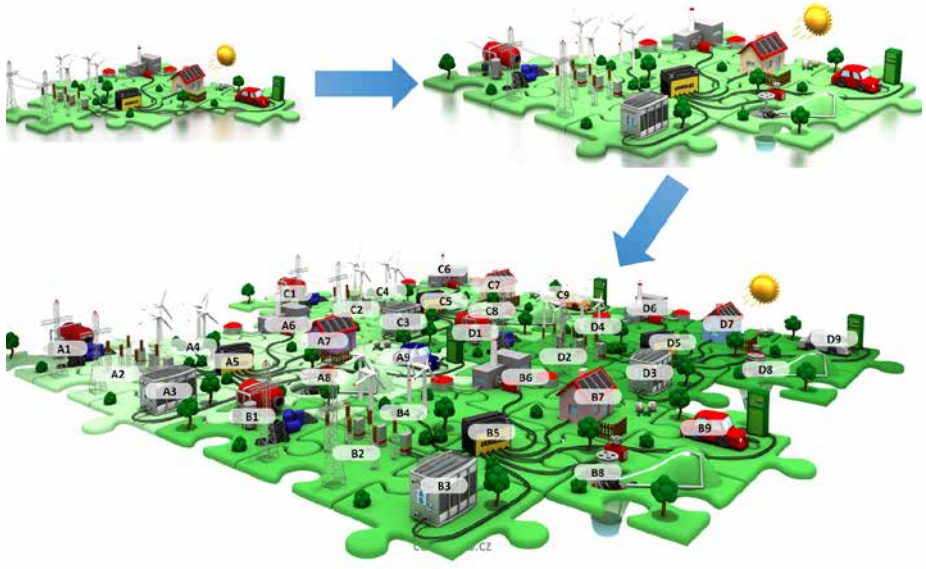
In May last year, a strategic project called Energy System for Grids (ES4G) began. The ES4G project brings together a unique investigating consortium; ENET Centre and IT4Innovations at VSB-TUO, and Brno University of Technology, along with application guarantors E.ON Distribuce, a.s., ČEZ Distribuce, a.s., and ABB s.r.o. They act as mentors and direct the focus of the project's research activities with regard to the strategic direction of the energy industry.

The aim of the ES4G project is the development of a new system solution for energy flow control in the energy platform of a Sophisticated Energy System (SEN) on the level of distribution networks, to supply energy platforms of municipalities, towns, and microregions. SEN will be supported by sophisticated control methods and prospective technologies to increase its security, reliability, raw material self-reliance, and energy self-sufficiency, while maximizing the exploitation of decentralized, particularly renewable sources of energy. This way, the project aims at ensuring the readiness for a change in the energy system control concept having implemented the EU Winter Package in compliance with the National Action Plan for Smart Grids and the State Energy Conception.

Role of IT4Innovations in the ES4G project

Pavel Praks, who is involved in the project solution within IT4Innovations, explains the cooperation with the ENET Centre: *"We are developing a model of the electricity distribution network in the Czech Republic. The focus of the research team from the Advanced Data Analysis and Simulations Lab is to optimize and validate the electric grid model, including testing the numerical reliability and robustness of the methods. Analyses will also focus on modeling individual failures and their combinations to describe the impacts of these failures on the proper supply of electricity to customers."*

Because of the combinatorial explosion of states, the task is so computationally demanding that the solution cannot simply be quantified, even using a supercomputer. Therefore, biologically inspired algorithms are also used to optimize the operation of the electricity network. The Pandapower software is used for modeling, and stochastic algorithms, namely genetic algorithms, particle swarm optimization, and simulated annealing are used for verification. IT4Innovations is in the process of testing the speed, accuracy, and reliability of these approaches, and the ongoing work process and results are being consulted with the project partners, including the application guarantors.



New software development for ES4G

IT4Innovations develops software to identify critical components of the electrical grid. Various normal and abnormal operating states are simulated in the grid model, and the effects of these states on network elements and their surroundings are monitored. The aim is to identify combinations of electrical grid components that, if they fail, lead to major changes in power flow or to network failures. The knowledge gained of critical components will also be used to facilitate the modeling of fault scenarios, and to obtain information on bottlenecks in networks to increase the robustness of the network.

At IT4Innovations, the prediction software package aimed at predicting the power consumption of the energy system from data is currently being developed. The new AI Feynman software is being tested using Nvidia GPU graphics cards and prediction methods based on decision trees (e.g., XGBoost). IT4Innovations is also active in the development and testing of algorithms for qualifying and quantifying the properties of dynamic systems, thus approximating entropy, maximal Lyapunov exponent and the 0-1 test for chaos applied to numerical simulations performed with supercomputers.

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Project No. TK02030039 Energy system for grids is co-financed by the Technology Agency of the Czech Republic under the THETA: Funding Program for Applied Research, Experimental Development and Innovation.

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EVEREST PROJECT

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IT4Innovations participates in the prestigious EVEREST project

IT4Innovations National Supercomputing Center has officially started cooperation in the international EVEREST project. Within this project, the Czech Republic collaborates with nine other partners from five European countries. The role of Principal Investigator for the project for IT4Innovations, which is funded by the Horizon 2020 framework program, will be performed by Kateřina Slaninová from the Advanced Data Anaysis and Simulations Lab.

The distributed and heterogeneous nature of the data sources in High Performance Big Data Analytics (HPDA) applications, as well as the required computational power, are the aspects pushing designers towards novel computing systems that combine high performance computing (HPC), Cloud services, and IoT solutions with Artificial Intelligence (AI) algorithms. *"The EVEREST project focuses on finding a match between application requirements and the characteristics of the underlying hardware system, because only an optimal match leads to efficient computation. In particular, we forecast that future systems will not only reflect requirements based on data, but will also feature complex architectures that must be redesigned and customized based on the nature and locality of the data, and the type of learning or decisions to be performed,"* explains Kateřina Slaninová.

The EVEREST project aims to develop a holistic approach for co-designing computation and communication in a heterogeneous, distributed, scalable, and secure system for HPDA. This is achieved by simplifying the programmability of heterogeneous and distributed architectures through a "data-driven" design approach, the use of hardware-accelerated AI, and through efficient monitoring of the execution with a unified hardware-software paradigm. The EVEREST project proposes a design environment that combines state-of-the-art programming models and emerging communication standards with novel and dedicated domain-specific extensions.

In order to validate the proposed approach within the EVEREST project, three application scenarios will be used, with each focused on a particular industry: a weather analysis-based prediction model for the renewable energy trading market, an application for air-quality monitoring of industrial sites, and a real-time traffic modeling framework for intelligent transportation in Smart Cities.

"IT4Innovations and the company Sygic will be responsible for the third application scenario mentioned, which models traffic in real time. Apart from this, we will also be ensuring the technical part, engaging in the further development of programming models for the orchestration of complex workflows, and exploitation and dissemination of the results emerging from within the project," specified Kateřina Slaninová. *"Traffic modelling based on large amounts of data using advanced AI technologies seems to us to be a forward-looking way to develop relevant transport solutions for cities. We believe that this project and collaboration with IT4Innovations will help us bring such solutions to the market,"* said Radim Cmar, Solution Architect at Sygic.

EVEREST PROJECT

- 2019–2023
- Funded by the European Union Horizon 2020 Research and Innovation Program
- Total budget is EUR 5,037,372.50
- The Project Coordinator is IBM Research GmbH from Switzerland
- 10 partners: IBM Research GmbH (Project Coordinator), Politecnico di Milano, Universita della Svizzera Italiana, Technische Universität Dresden, Centro Internazionale in Monitoraggio Ambientale, IT4Innovations, VSB – Technical University of Ostrava, Virtual Open Systems SAS, Duferco Energia Spa, Numtech, Sygic a.s.

For more information, see here.

SYGIC COMPANY

Developed in Bratislava in 2004, Sygic is a leading developer of mobile offline GPS navigation apps for regular customers, corporate fleets as well as professional drivers. Sygic has also developed its own map and navigation platform to process data for intelligent transport called the Smart Mobility Platform.

For more information, see the website.

This project received financial support from the European Union Horizon 2020 Research and Innovation Program under Grant Agreement No. 957269.

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EVENTS HELD IN AND WITH OUR CENTRE

THE 4TH IT4INNOVATIONS USERS CONFERENCE WAS HELD VIRTUALLY

We, too, are keeping up with the times, and so, on 5th November 2020, the 4th IT4Innovations Users Conference was held in a completely virtual format. Despite the online format, 68 guests attended! The conference provided information on the plans we are making for infrastructure as well as new services related to our involvement in the e-INFRA CZ, or LUMI consortium. The conference was conducted by Branislav Jansík, IT4Innovations Supercomputing Services Director, and Jan Heyda of the Institute of Physical Chemistry of the University of Chemistry and Technology in Prague and the Chairman of the IT4Innovations Users Council.

There were four keynote lectures given by our users, which were selected by the Program Committee:

- Dominik Legut (IT4Innovations) “Lattice vibrations and the trimerons order of magnetite at Verwey transition”
- Jiří Klimeš (Faculty of Mathematics and Physics of Charles University in Prague) “Precision in ab initio calculations”
- Michalis Kourniotis (Astronomical Institute of the Czech Academy of Sciences) “Multiple Stellar Generations Within Globular Clusters”
- Petr Strakoš (IT4Innovations) “Research and development of an input data generator for obstacle detection training in a simulated environment”

In the poster section, 19 posters from various scientific fields were presented.

For posters, see HERE.

SUPERCOMPUTING CONFERENCE SC20

The online SC20 conference opened its virtual gates from the 9th to the 19th of November. Even this year, IT4Innovations could not help but participate among the exhibitors despite having only a virtual booth. Jakub Beranek and Stanislav Böhm of IT4Innovations presented their contribution entitled “Runtime vs Scheduler: Analysing Dask‘s Overheads” within the workshop section on 11th November.

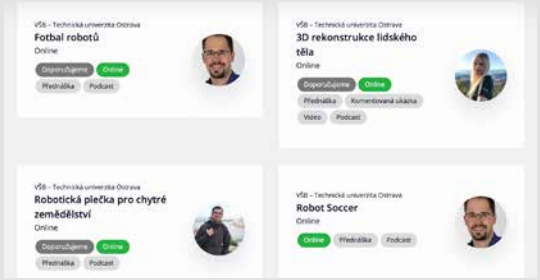
For presentation, see HERE.

At the Supercomputing Conference, the TOP500 list of the world‘s most powerful supercomputers was announced. The winner is again Japan‘s Fugaku. Even after 5 years of operation, our Salomon is still in the rankings, although it has fallen to 462nd place. Are you also curious how well Karolina, which is to be launched this year, will perform?

For the latest TOP500 list, see here.

LISTEN TO THE PODCASTS FROM RESEARCHERS’ NIGHT

The biggest event held at the IT4Innovations premises dedicated to the general public has also been given in an online format. The usual attendance for this event is around 700 participants. In order not to deprive those interested in the latest development in research carried out in our centre, we have prepared interesting podcasts. Listen to them too. Václav Svatoň will give you an overview of what Robot Football looks like, Petra Svobodová will tell you why the future of medicine is in 3D visualization and virtual reality, and Jakub Beránek will answer the question of how a smart agricultural machine of the 21st century works.



Robot football

3D human body/anatomy reconstruction

Robotic smart agriculture weeding machine

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