NEWSLETTER Q4/2019

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

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IN BRIEF

19TH OPEN ACCESS GRANT COMPETITION

You can apply for IT4Innovations computational resources within the 19th Open Access Grant Competition from **5th February 2020.**

www.it4i.cz

PUBLICATION

System-Scenario-based Design Principles and Applications publication

With their Run-Time Exploitation of Application Dynamism for Energy-Efficient Exascale Computing chapter, Ondřej Vysocký and Jan Zapletal from the Infrastructure Research Laboratory contributed to the System-Scenario-based Design Principles and Applications book published by Springer Nature.

For more details about book

RECOGNITION IN THE VISIONARIES 2019 PROJECT COMPETITION

In early December, the implementation team led by Prof. Zelinka from VSB-TUO and our colleagues from the Big Data Analysis Laboratory received an honorary award from the expert panel within the Visionaries 2019 project competition for their Chiméra mobile application for encrypted communication. The Visionaries 2019 project competition was held under the auspices of the Ministry of Industry and Trade of the Czech Republic and the Technology Agency of the Czech Republic.

For more information about Chiméra

BARBORA KACEROVSKÁ

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

THE WINNER OF THE HPC AMBASSADOR AWARD – PRACE SUMMER OF HPC 2019

Our guest during PRACE SoHPC, Pablo Llunch Romero received the Ambassador Award – PRACE Summer of HPC 2019 for his “Emotion Recognition using Deep Neural Networks project.” Congratulations to Pablo and his mentor Georg Zitzlsberger. For the video presentation of the winning project, SEE

For more about the award ceremony

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THE AGREEMENT ON HOSTING THE PETASCALE SYSTEM AT IT4INNOVATIONS SIGNED

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At the end of November last year, a formal meeting bringing together the representatives of the countries to host European pre-exascale and petascale systems in 2020 was held in Strasbourg, Germany. IT4Innovations National Supercomputing Center was, of course, one of them. The central purpose of the meeting was the signature of the hosting agreements between the EuroHPC Joint Undertaking and each of the hosting centres, where these computing systems are to be located.

The names of the eight European institutions which were selected for hosting the new pre-exascale and petascale systems were announced in June 2019. The systems with pre-exascale power are to be located in the supercomputing systems in Spain (BSC), Italy (CINECA), and Finland (CSC), where IT4Innovations participates as a member of the LUMI consortium, and as such, it shall also be involved in operation of this new pre-exascale system. Five additional petascale systems are to be located. It is system which is to be also installed at IT4Innovations National Supercomputing Center in 2020, among others. The other successful candidates include Bulgaria (Sofiatech), Luxembourg (Luxprovide), Portugal (Minho Advanced Computing Centre), and Slovenia (IZUM).

The signed hosting agreements are contractual documents that define the roles, rights, and obligations of each hosting centre. The procurement process for the eight new supercomputers can now begin. The petascale and pre-exascale supercomputers are expected to be put into operation in the middle of the year 2020 and during the year 2020, respectively.

On behalf of IT4Innovations National Supercomputing Center, Branislav Jansík, the Supercomputing Services Director, participated at the meeting in Strasbourg. *„The hosting agreement signature is the first important step towards procuring the petascale system that will be located at IT4Innovations. The process of preparing the mandatory public procurement documents for this system has already been set in motion so as to locate it in our centre by the end of the year 2020,"* says Jansík

These new supercomputers will be made accessible to European researchers as well as industrial enterprises to develop new applications in areas such as artificial intelligence, material sciences, the pharmaceutical industry, bio-engineering, weather forecasting, and combatting climate change.

"The signature of these hosting agreements marks a milestone in the Joint Undertaking's activities, bringing us a step closer to our ambition of making Europe a global leader in high performance computing. By the end of next year, eight world-class supercomputers will help European researchers and industry, wherever they are in the EU, run applications that require large amounts of computing power to make significant advances in fighting climate change, designing new drugs, developing new materials, and many other areas. I also welcome North Macedonia as the Joint Undertaking's thirtieth member. I am delighted that, as part of its engagement with the EU's Digital Agenda for the Western Balkans, the country has committed to investing in the Joint Undertaking and in its ambitious infrastructure and research objectives," said Mariya Gabriel, the European Commissioner for Digital Economy and Society.

Branislav Jansík and Mariya Gabriel celebrating the official signature of the agreement on hosting the petascale system at IT4Innovations.

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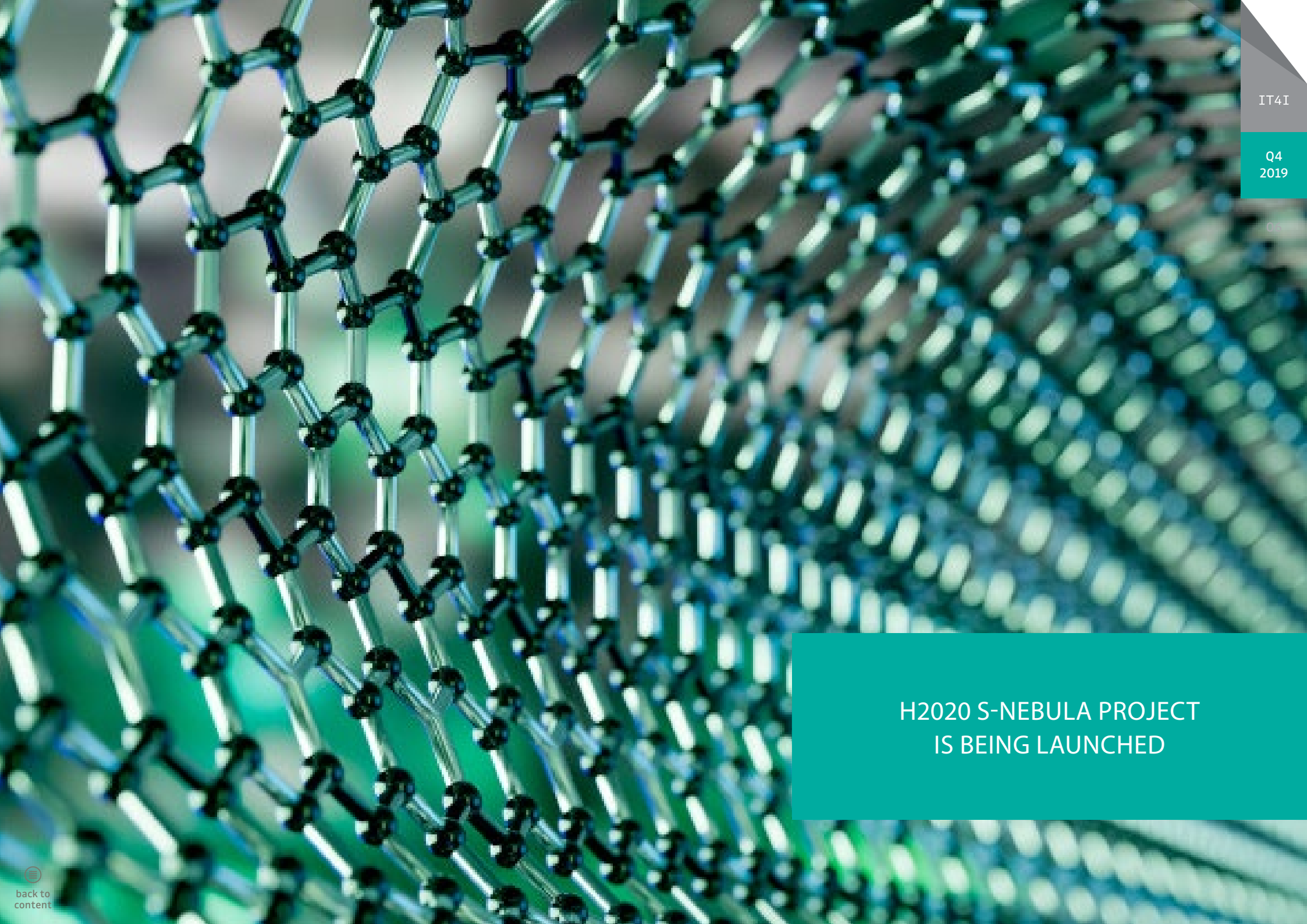

H2020 S-NEBULA PROJECT IS BEING LAUNCHED

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H2020 s-NEBULA project is being launched

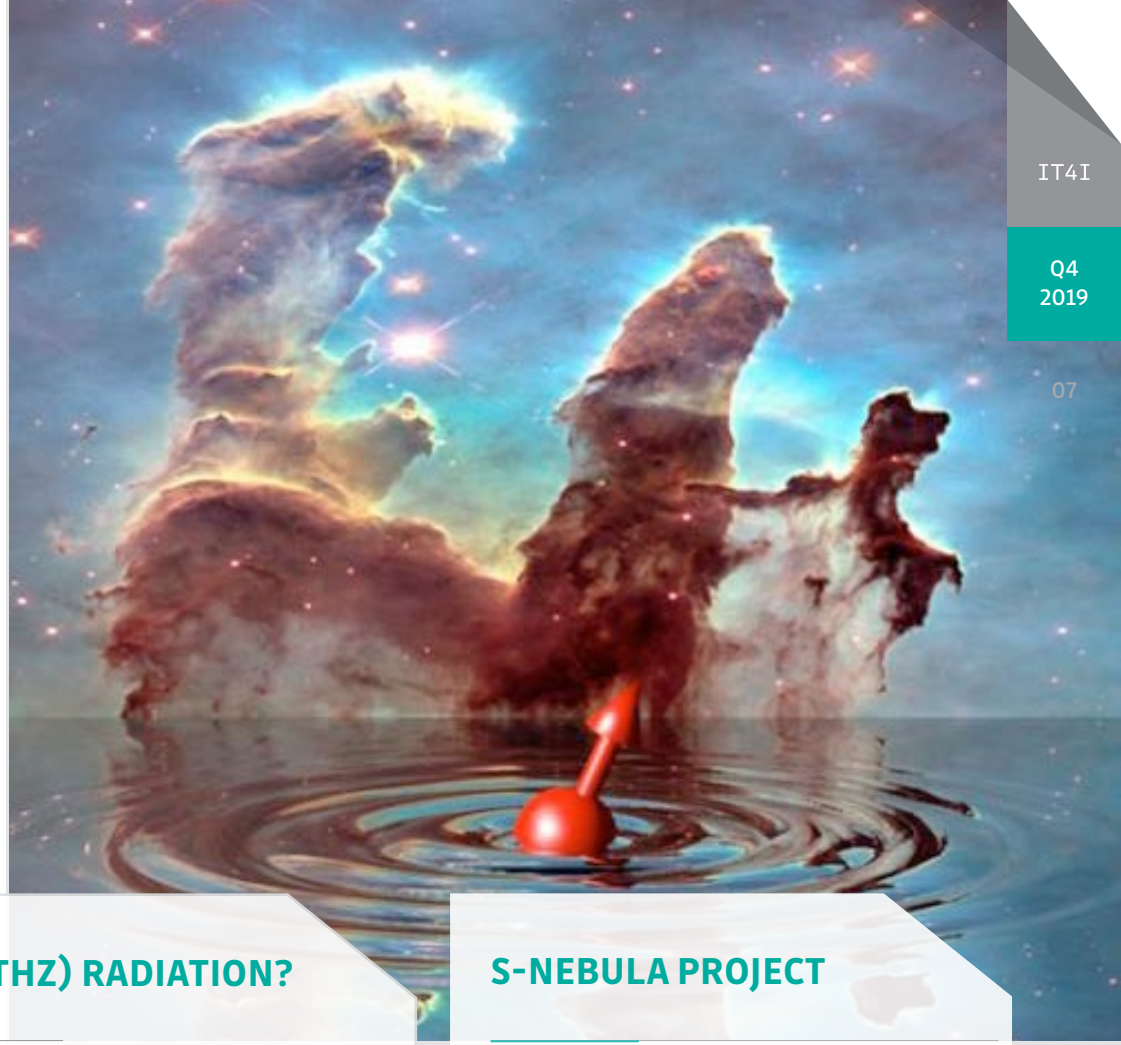
At the beginning of the year 2020, the s-NEBULA project was launched, aiming to develop new methods and technology using spin electronic properties for advanced Terahertz spectral range-based applications.

The researchers of IT4Innovations and the Nanotechnology Centre are commencing work on the next Horizon 2020 project. In the new s-NEBULA (Novel Spin-Based Building Blocks for Advanced TeraHertz Applications) project, our colleagues from the Modelling for Nanotechnologies Laboratory will be involved in the research and development of the revolutionary approach to terahertz (THz) technologies using spin for both generation and detection of THz radiation.

The s-NEBULA project ambition is to provide a platform for new THz technologies based on innovative combination of magnetism and optics. This project shall provide cutting-edge solutions to scientific problems in the field of technologies using THz radiation, such as broadband pulsed and continuous-wave emitters and voltage-controlled compact detectors for non-destructive testing (NDT), pulse and continuous-wave emitters for THz communication, and polarization-programmable emitters for THz ellipsometry.

The s-NEBULA project will also focus on research of new antiferromagnetic materials with direct voltage rectification effects targeting a tunable and compact detector, which is the key element for on-chip THz systems. On top of that, the combination of THz radiation and magnetism shall enable the emitted waves to be controlled, performing intrinsic modulation and demodulation as well as polarization control of radiation sources in ellipsometry.

"The above-mentioned approaches cannot be effectively applied with the existing THz radiation knowledge. Therefore, development of the new platform using electron spin is crucial for future THz radiation-based technologies," said Prof. Jaromír Pištora, the Head of IT4Innovations Modelling for Nanotechnologies Laboratory.



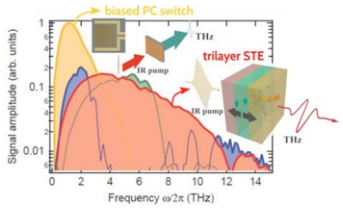
WHAT IS TERAHERTZ (THZ) RADIATION?

THz refers to an electromagnetic spectrum range within the microwave and infra-red radiation band. The electromagnetic wave frequency ranges from 0.3 THz up to 3 THz, with the corresponding wavelengths of radiation in the terahertz band being lower than 1 mm and higher than 100 μm. THz technologies are used in spectroscopy, non-destructive testing, security technologies, biology and medicine, astronomy, and high-speed, high-capacity broadband telecommunications.

For more detail about THz radiation

S-NEBULA PROJECT

- 7 partners from 4 EU membership countries
- Implementation period of 3 years
- Budget of EUR 3.4 million
- This project is funded from the H2020-EU.1.2.1. programme, project ID 863155.



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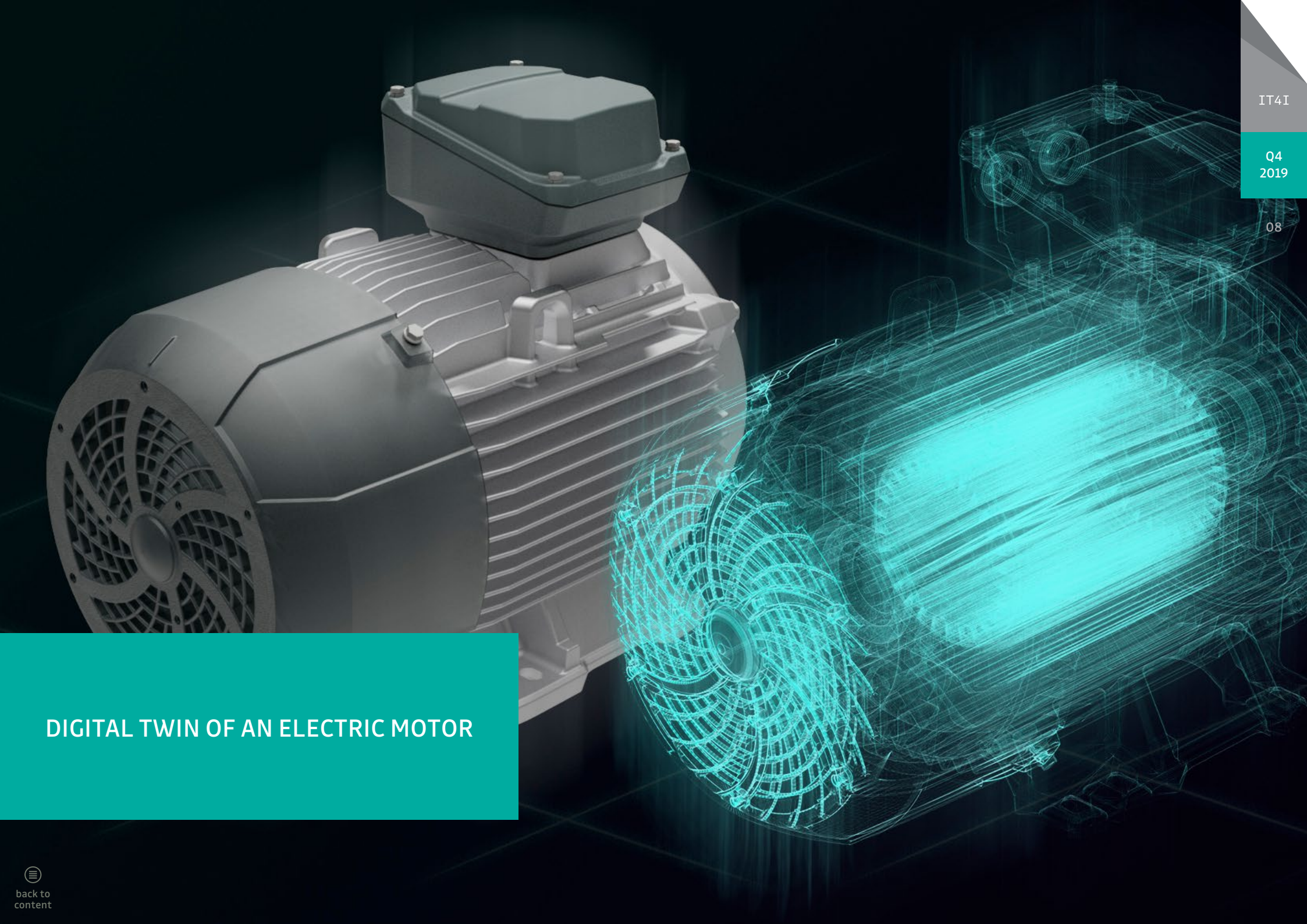

DIGITAL TWIN OF AN ELECTRIC MOTOR

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Digital twin of an electric motor

Since October 2019, IT4Innovations has been involved in implementing a project funded by the Ministry of Industry and Trade of the Czech Republic within the Operational Programme Enterprise and Innovation for Competitiveness (MIT OPEIC) – Application in cooperation with Siemens, s.r.o., as the main beneficiary as well as Elektromotory Frenštát and SVS FEM s.r.o. companies. The project objective is research and development in fields closely related to production digitalization and design of a digital twin of an electric motor. This digital twin is a complex digital representation of a product allowing the production and innovation cycle to be increased and shortened, respectively. In a virtual environment, it is possible not only to create prototypes but also simulate their functionality and operating parameters. The key feature of this technology is the digitalization of a product, its production process, as well as putting a given product into operation. Employment of high-performance computing in the design and operation of the digital twin is one of the crucial factors affecting the practical applicability of the digital twin technology. Using tools for simulation, testing, and optimization of processes, companies are enabled to create a digital twin and thus smooth all details and debug all potential errors of a given machine before it is put into operation. Collection and evaluation of data during operation enable the processes to be continually monitored, and maintenance and service costs to be predicted in real time.

Now is the time for companies wishing to retain their competitiveness and market position to take the first steps towards digitalization. Digitalization is a promising trend in terms of cost reduction as well as production quality, flexibility, and efficiency increase. It allows companies to respond faster to ever increasing and more individualised requirements of customers, and opens up opportunities for new and innovative areas of business activity. Due to growing requirements of customers as a result of new communication technologies, the pressure on development and supply of products in a fast, high-quality, customised manner is increasing, even if in mass production. Investment in digitalization is of crucial importance for the growth of all industrial companies regardless of their size or area of activity. Enterprises need to reduce the time to market their products and enhance flexibility and efficiency with higher quality guarantees. These requirements cannot be met by mere implementation of automated production processes. Digitalization is particularly promising in industrial production, which needs to be tackled with a complex approach comprising the entire value chain, including suppliers. Such approach allows the entire development and manufacturing processes to be digitalised, starting from the product design and preparation, to production design and it's putting into operation, operation, and modernisation of machinery as well as production facilities. This is the only way to reap the full benefits that digitalization can deliver.

SIEMENS

Digital twin Siemens

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IT4INNOVATIONS DIGITAL INNOVATION HUB

IT4Innovations Digital Innovation Hub

DIH OSTRAVA

An integral part of the IT4Innovations activities is its cooperation with industry, for which IT4Innovations was earlier awarded the status of the Digital Innovation Hub registered at the European Commission level. At the beginning of the year 2020, a memorandum about the key partnership between IT4Innovations and the Moravian-Silesian Innovation Centre (MSIC) will be signed to set up the Digital Innovation Hub Ostrava (DIH Ostrava), which shall play an important role in supporting the development of digitalization in small and medium-sized enterprises in the Moravian-Silesian Region and other regions.

Digital Innovation Hubs are based on regional cooperation among partners such as research organizations, industrial associations, incubators/accelerators, and particular enterprises. It is in this context that the Digital Innovation Hub Ostrava is being established and integrates the know-how of both partners, IT4Innovations and MSIC, with the objective toprovide a complex portfolio of complementary services in the field of digitalization, including individual consultancy services, use of high-performance computing, computer simulations and modelling, augmented virtual reality, and artificial intelligence.

We have asked Martin Duda, the DIH Ostrava Coordinator for IT4Innovations, about the DIH Ostrava activities.

What are the primary benefits you expect from the cooperation established between IT4Innovations and MSIC within the currently developing DIH Ostrava?

"Both entities have acquired very interesting know-how, which we strongly believe will have a significant synergic effect. MSIC is apt to identify and establish cooperation with enterprises exhibiting innovation potential and to provide them with customised support including implementation of digital innovation. IT4Innovations, on the other hand, is apt to provide such support in specific areas of digitalization such as high-performance computing, big data analysis, and artificial intelligence."

What is the position of DIH Ostrava in the context of the Czech Republic?

"I dare say it is unique. This, in my opinion, lies in the fact that IT4Innovations is a unique infrastructure in the Czech Republic. Moreover, it has the potential to offer interesting opportunities to enterprises. MSIC, on the other hand, is one of those regional innovation centres which have managed to build trust and reputation for its ability to help enterprises in their development. Not only in the Czech Republic but also in the EU, there are only few regions which can boast having theira digital innovation hub with a composition such that they can provide state-of-the-art technological capacity (infrastructure and know-how) on one hand and a pro-active innovation centre dealing with companies on a daily basis on the other hand, with both parties sharing the vision to support digitalization in the business sector."

Is the situation in Europe comparable?

"The composition of digital innovation hubs in each EU member state shall differ to some extent, particularly depending on their institutional environment. For example, in Germany and southern Europe it can be expected that Frauenhofer institutes as centres for applied research and clusters or business associations, respectively, will play an important role in this area."

How can industrial enterprises access the computational resources of IT4Innovations?

"One of the ways is to participate in joint research projects with IT4Innovations, which are mostly publicly co-funded. Another way is to be provided contract research services, including allocation of required computational resources. We are currently launching - as part of the pilot testing of the DIH Ostrava concept – a special offer of funding this form of access as an affordable service for small and medium-sized enterprises. We are aiming to attract innovative enterprises that would otherwise have no means to pay the full cost price of computational resources used. Last but not least, enterprises may go for standard renting of the computational resources."

Are there any European Union projects helping small and medium-sized enterprises access computational resources?

"Yes, there are. One of them is PRACE SHAPE, which not only provides computational resources but also expert consultations. Another such project is CloudiFacturing, which offers development of customised solutions for enterprises. CloudiFacturing is a cascade-funded project, which means that there is a project consortium deciding the allocation of funds for particular cases with a third

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party, such as a supercomputing centre and an enterprise, being involved in project solution implementation. It can be expected that this kind of support will be provided through a relevant DIH or EuroHPC JU in the future."

The development of DIHs is also one of the most important pillars of the European Commission within the industrial initiative for a single digital market. IT4Innovations is a member of the European network of digital innovation hubs, namely DIHNET EU and as such it was awarded DIH of the month for its activities in November 2019.

We have spoken with Tomáš Karásek, the Head of the Parallel Algorithms Research Laboratory, about IT4Innovations' cooperation with industrial enterprises.

What are the particular services IT4Innovations most frequently provides nowadays?

"As mentioned above, IT4Innovations provides services to industrial enterprises in several ways. They can rent the computational resources with or without IT4Innovations' support. Such support includes installing codes on clusters, running codes on clusters, HPC consultations, etc. Another way is to use knowledge and skills of IT4Innovations researchers through contract and collaborative research.

IT4Innovations has ampleexperience with development and optimization of parallel codes for HPC architectures (GPU, Xeon Phi). The code optimization experience is further reinforced by both methods and tools as part of our participation within the POP2 Centre of Excellence programme. Our experts have hands-on experience with BSC tools for optimisation (Extraw, Paraver, Dimemas, etc.) and JSC tools based on Score-P (Scalasca, Cube, Vampir, etc.). Additionally, IT4Innovations has experts capable of code analyzation using commercial tools such as Intel (VTune Amplifier), and ARM (MAP, Performance reports).

Another important activity directly associated with IT4Innovations computer technology consists in organizing training and workshops. IT4Innovations organizes more than ten seminars and conferences annually, where presentations of leading, often foreign lecturers and experts can be heard. Since the launch of its operation in 2013, IT4Innovations has organized 63 high-quality educational and training events, as well as six seasonal schools. IT4Innovations training events are free of charge, open to the public, and are designed to demonstrate utilization of the operated supercomputers."

Can you give us a practical example of an innovative solution developed in cooperation with IT4Innovations?

"Throughout IT4Innovations' existence, we have collaborated with industrial companies within a number of interesting projects. One of them was a collaboration project with the BORCAD, which produces railway passenger seats. In order to place their products on the UK market, their seats had to comply with enormously strict safety criteria including a safety certificate, which could only be obtained after passing seat crash tests. These crash tests are not only expensive but also time-consuming, as a prototype must be first created and then tested. Numerical modelling and simulations of the above-mentioned crash tests are one of the most practical and frequently used methods, which are rather hard to perform for small and medium-sized enterprises in technical and temporal terms.

For these above-mentioned reasons, BORCAD turned to IT4Innovations, which has both HPC resources and highly-skilled research staff, and we jointly set up a scientific team. The existing construction cycle was adjusted so the entire construction and its changes were first tested, and only after that subjected to a physical crash test performed by a certified laboratory. In 2016, this project, entitled improved passive safety and comfort of passengers in railway traffic, won the Technology Transfer Award."

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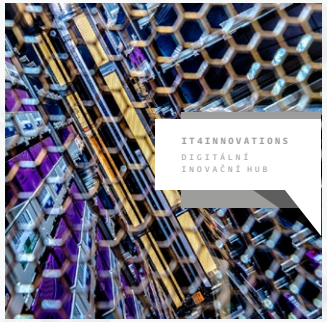
WHAT DIGITAL INNOVATION HUBS STAND FOR

Digital Innovation Hubs (DIHs) serve as a supportive instrument to help companies become more competitive through improvement of their business/production processes, products, and services using digital technologies. DIHs work as one-stop-shops, which help companies in digitalizing their business.

DIHs provide access to knowledge and technologies that are normally unavailable to the commercial sector. With their assistance, companies have an opportunity to experiment with these digital innovations, which in turn may simplify their decision making as well as implementation of these technologies and know-how in their business structures. Main DIH clients include small and medium-sized enterprises, public administration institutions, and medical centres, all of whom contribute to the enhancement of the life of society as a result of implementing these digital innovations.

COOPERATION WITH INDUSTRIAL ENTERPRISES

Since 2012, IT4Innovations has collaborated with more than 60 enterprises in 120 research projects amounting to EUR 1.1 million. In the last 3 years, these enterprises rented more than 10 million core hours. For more information, please see the Digital Innovation Hub brochure.



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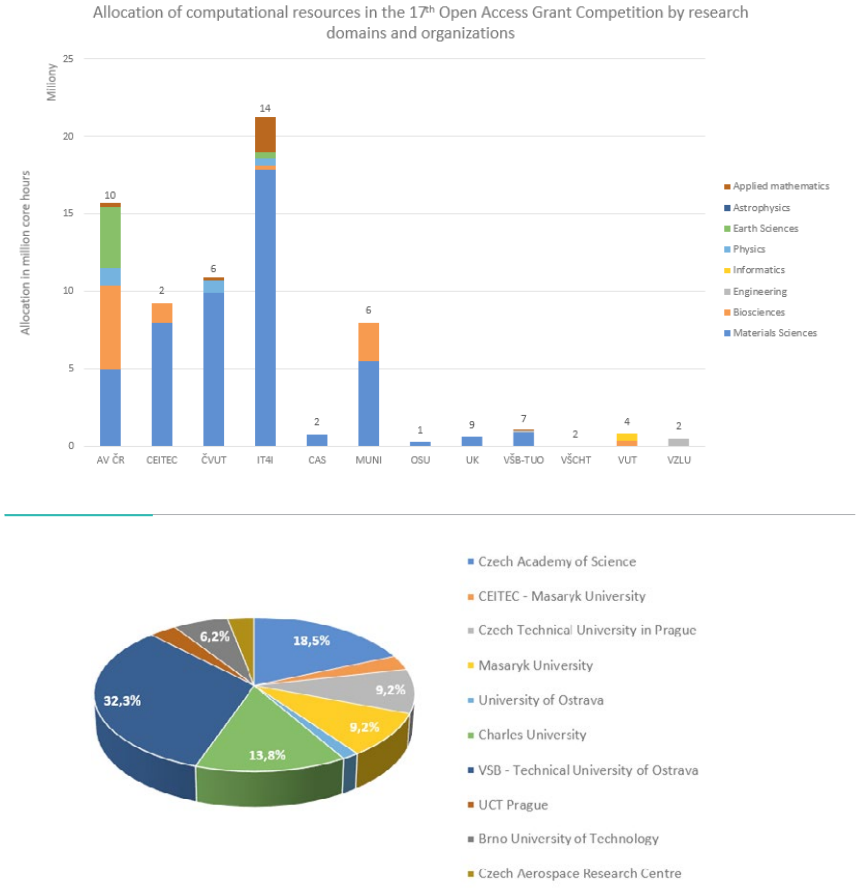
EVALUATION OF THE 17TH OPEN ACCESS GRANT COMPETITION

In the 17th Open Access Grant Competition (OAGC), the interested candidates applied for more than 116 million core hours within the standard nine-month access. The excess of demand over the increased reserved capacity for this OAGC (66 million core hours) was 75 %. Therefore, the Allocation Committee decided to lower the allocations of the evaluated projects as well as to increase the allocated core hours. In this OAGC, the Allocation Committee thus distributed 85 million core hours across 65 successful projects, with 7 of them being multi-year projects.

Most of the allocated core hours, i.e. almost 22 million core hours (32 % of the total distributed computational resources) were awarded to researchers from VSB-TUO for their 21 projects. Czech Academy of Sciences institutes were awarded about 16 million core hours (18.5% of the total distributed computational resources) for 12 projects. Last but not least, Charles University in Prague was awarded 15.5 million core hours (13.8 % of the total distributed computational resources) for their 9 projects.

Other institutions being awarded the computational resources in the 17th Open Access Grant Competition for implementing their research projects include Masaryk University in Brno, CEITEC, the Czech Technical University in Prague, the University of Ostrava, Brno University of Technology, the University of Chemistry and Technology Prague, and the Czech Aerospace Research Centre.

Allocation of more than 1 million core hours was awarded to each of the 26 projects led by researchers from Charles University in Prague, the Czech Technical University in Prague, the Czech Academy of Sciences, Masaryk University in Brno and VSB – Technical University of Ostrava. The first three most successful projects were awarded a total of 21 million core hours. Nearly 8 million core hours and more than 7 million core hours of our computational resources were awarded to Prof. Mojmír Šob from CEITEC and doc. Dominik Legut from IT4Innovations based at VSB-TUO, respectively. The third highest allocation of more than 6 million core hours was awarded to Prof. Petr Nachtigall from Charles University in Prague, for his project entitled Stability of Zeolite Catalysts in the Presence of Water.



Allocation of computational resources in the 17th Open Access Grant Competation by research domains and organizations

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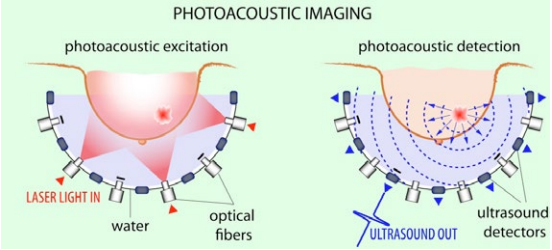
WE INTRODUCE SELECTED PROJECTS WHICH WERE AWARDED OUR COMPUTATIONAL RESOURCES IN THE 17TH OPEN ACCESS GRANT COMPETITON:

Dr Jiří Jaroš
(Brno University of Technology)

PHOTOACOUSTIC TOMOGRAPHY OF THE BREAST

Jiří Jaroš from BUT was awarded more than 300,000 core hours for validation of the developed photoacoustic tomography (PAT) software on a set of breast phantoms and optimisation for speed and accuracy. The goal is to validate the generated PAT image under noisy conditions and the presence of moving artifacts, inhomogeneous lighting, limited sensor bandwidth, and variability between ultrasound sensors caused by a given production technology. This data will be used for fine tuning of the PAT software before being used with a set of 20 patients. The images generated using photoacoustic tomography, x-ray imaging, and computed tomography will then be passed on to clinical doctors for evaluation. The results of this study shall lead to development of new screening and diagnostics methods in breast mammography.



Photoacoustic imaging process

The tissue is exposed to an infrared beam with a nanosecond pulse with energy being absorbed by tumour blood vessels. Then, thermo-elastic expansion occurs inside the tumour (the tumour trembles). Radiation changes into heat in the form of generating ultrasound pulses by density change. Ultrasound propagates out of the tissue and is recorded on the surface of ultrasound detectors. The goal of these simulations performed within the project is to use the recorded signal to reconstruct the place the sound comes from, and its quantitative qualities (position of blood vessels, their size, amount of oxygenated blood, etc.).

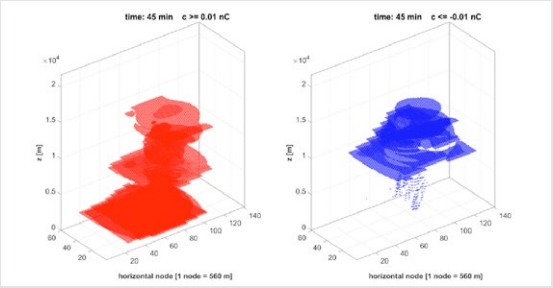
Dr Zbyněk Sokol
(Institute of Atmospheric Physics CAS)

ELECTRIFICATION OF THUNDERSTORMS

simulations of selected events

More than 1 million core hours was awarded to Zbyněk Sokol from the Institute of Atmospheric Physics CAS for simulation and study of electrification of thunderstorms. Thunderstorms are one of the most dangerous climate phenomena, which are accompanied with strong gusts of wind, hail, and high lightning activity. Although they can lead to huge socio-economic losses related to severe material damages as well casualties, thunderstorms have not been fully described and understood yet, which makes their prediction uncertain. One of the processes in thunderstorms that remain unclear is the process of electrification.

Zbyněk Sokol, together with his colleague Jana Minářová, will use the supercomputer to simulate the electrification process during convective thunderstorms which were observed within the territory of the Czech Republic between 2018 and 2019. These simulations will take place using the Cloud Electrification Model (CEM), which has been implemented in the COSMO Numerical Weather Prediction model, or CEM-COSMO. The authors consider their project innovative as it is the first time that electrification of thunderstorms will be studied over the territory of Central Europe. The project results may lead to expanding the knowledge related to thunderstorms, such as electrification and lightning activity, as well as more accurate weather forecast modelling.



Simulation of a thunderstorm using the CEM-COSMO model (Cloud Electrification Model implemented in the COSMO NWP model).

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Dr Lubomír Rulíšek
Institute of Organic Chemistry and Biochemistry CAS

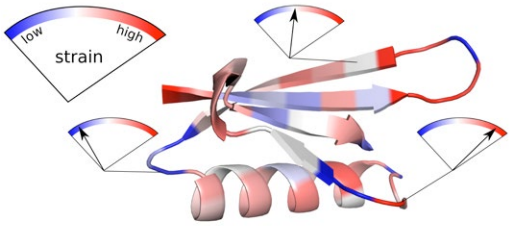
CONFORMATIONAL BEHAVIOUR OF SMALL PEPTIDE FRAGMENTS STUDIED BY QUANTUM CHEMICAL METHODS

To what extent does conformational strain in proteins determine their three-dimensional structure? This is a question Lubomír Rulíšek from the Institute of Organic Chemistry and Biochemistry CAS is aiming to answer using the more than 5 million core hours he was awarded.

Large-scale quantum chemical calculations coupled with modern solvation methods represent a unique set of ab initio tools to explain the key determinants of biomolecular structure. Understanding the conformational strain in proteins and in their ligands may represent a new and computationally tractable way to significantly deepen our understanding of protein folding and of protein-ligand interactions.

The aim of this work is to determine the conformational space of all 400 existing dipeptides and the energy map of the conformers. Based on this large dataset, it is then possible to understand the trends and rules determining the spatial structure of proteins.

Apart from the computed data, Lubomír Rulíšek with his colleagues Martin Culka and Tadeáš Kalvoda will perform experimentally-verifiable sets of tests, which shall provide evidence for the proposed hypotheses. The project results shall find their area of application in, for example, the design and development of drugs as well as the design of specific enzyme-based catalysts.

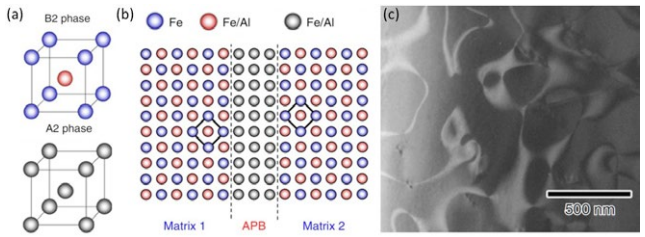


Prof. Mojmír Šob
CEITEC

FROM ANTIPHASE BOUNDARIES TO NEW RARE-EARTH-FREE MAGNETS

The research team led by Prof. Mojmír Šob from CEITEC was awarded more than 8 million core hours for the project focused on analysis of antiphase (AP) boundaries on magnetic properties of intermetallic compounds and their thermodynamic as well as mechanical stability. This information is essential for successful development of new magnetic materials. The project aims at Fe-Al alloys, the magnetic properties of which can be improved by AP boundaries by up to dozens of per cents according to the latest experiments.

The awarded computational resources will be used by the research team to study the properties of conventional (rare-earth-free) Fe-Al-based magnets and to understand the relevant physical mechanisms, the knowledge of which is essential to improve the properties of these magnetic materials.



(a) The B2-type ordered phase without AP boundaries and A2-type disordered phase, which occurs on AP boundaries,

(b) The AP boundary separating the left B2-type ordered region (matrix 1) from the right B2-type ordered region (matrix 2). The APBs produced by the heat treatment show a finite width, of the order of nanometers,

c) Transmission electron microscopy (TEM) image revealing the locations of APBs (brighter features).

Source: the image was adapted from the work by Murakami et al.: Nature Comm. 5 (2014) 4133

APBs observed in the B2-type ordered Fe70Al30 alloy

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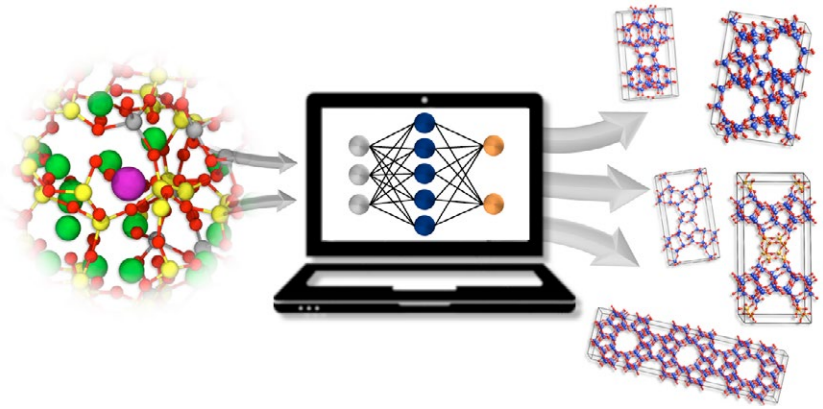
Dr Lukáš Grajciar
Charles University in Prague

NEURAL NETWORK POTENTIALS FOR IN SILICO DESIGN OF ZEOLITES

Lukáš Grajciar was awarded more than 2 million core hours for implementing his project focused on the in silico design of new catalysts, such as zeolites. Zeolites have great potential in the area of developing green technologies because they are the most important industrial catalysts used primarily in crude oil processing and petrochemistry. Lukáš Grajciar along with his colleagues Andreas Erlebach, Christopher J. Heard, and Petr Nachtigall use the awarded computational resources for simulations using deep neural network-based force fields for screening large databases of candidate structures and their modelling under operating conditions with unprecedented accuracy. The project results shall provide deeper insight into the structure and stability of existing and hypothetical zeolites, which have not yet been synthesized, and improve the catalytic properties of zeolites in general.



Neural network (middle), which is trained to match the material atomic structure (left) with the values of different properties such as values for their stability, and which allows for the design of materials with desired properties (right) once the training is finished.

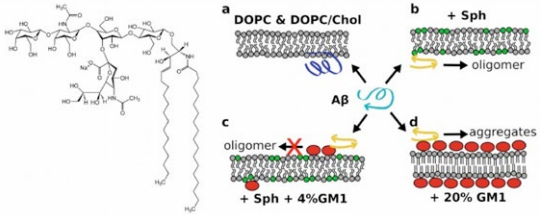
Dr Michael Owen
CEITEC

ALZHEIMER'S LIPIDS III

Alzheimer's disease is a chronic, progressive disorder of the nervous system, which causes degenerative death of neurons associated with characteristic histopathologic changes. This disease is diagnosed in 1 of 8 people aged over 65, which makes it the most common cause of dementia in middle-aged to upper-aged people. It is expected that by the year 2030, 14 million people will have suffered from this disease. Michael Owen from CEITEC was awarded over 1 million core hours for his first study, focused on the lipids associated with Alzheimer's disease. He will use the computational resources to shed light on the aggregation mechanism in amyloid-β (Aβ) peptide, which is a characteristic feature observed in Alzheimer's development and progression. Aggregation will be studied in the presence of gangliosides, which may affect Aβ peptide aggregation and have an undisputed role in the development and regeneration of the brain and progression of Alzheimer's disease.

Apart from gaining atomic insight into the role of gangliosides in Alzheimer's disease, this project will also be beneficial for the research of other neurodegenerative diseases such as Parkinson's and Huntington's diseases.

a) Aß does not oligomerise at DOPC and DOPC/Chol bilayers,
b) Oligomerisation of Aß is triggered by presence of sphingomyelin,
c) The binding of Aß to the headgroup of GM1 prevents its oligomerisation,
d) High density of both GM1 and Aß facilitates aggregation of the peptide and fibril formation explained by generic surface effects.



Left: Structure of the GM1 ganglioside.
Right: The proposed model reconciling Aß oligomerisation at membranes with various lipid composition.

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IT4INNOVATIONS USERS CONFERENCE WAS HELD FOR THE THIRD TIME

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3rd IT4Innovations Users Conference

The 3rd IT4Innovations Users Conference held at the beginning of November last year hosted more than 80 participants. For the first time, the conference was held as a two-day event and thus more time was given not only to the users' presentations but also for social networking. During the conference, 24 lectures and 3 keynotes presenting the research of IT4Innovations infrastructure users were heard. The speakers included representatives of IT4Innovations, the Czech Academy of Sciences, Charles University in Prague, CEITEC, the University of Chemistry and Technology in Prague, the Czech Technical University in Prague, and Masaryk University in Brno. The conference programme also included a Poster Section with 40 research project contributions being presented. Moreover, the IT4Innovations Users' Council was held as part of the conference.

The conference was opened by Branislav Jansík, IT4Innovations Supercomputing Services Director, who welcomed the participants and informed them about extending the infrastructure with the Barbora supercomputer as well as about future plans and development for the year 2020.

The first block of contributions was opened by Dominik Legut from IT4Innovations with his keynote presentation entitled 2D magnetic semiconductors – a power of HPC to predict. Using the Salomonsupercomputer for calculations, he investigates whether 2D magnetic semiconductors are suitable for use as ferromagnetic insulators in spintronic applications, such as large data storages, i.e. high-capacity hard disk drives.

The afternoon block was opened by Jiří Jaroš from Brno University of Technology, who presented his keynote on Ultrasound Simulation of Transcranial Neurostimulation. In his research work, he is involved in developing a tool covering the entire CT/MR screening process, from pre-surgical screening of a patient up to ultrasound application in a 3D-printed ultrasound device. The research results will be used in more accurate transcranial focusing, and prediction of intracranial fields using numerical simulation of ultrasound propagation in the heads of patients.

The second conference day was opened by Martin Matys from the Czech Technical University in Prague, who presented his Salomon-supported research project entitled Double layer target with interface modulations for laser acceleration of collimated ion beams. The project results shall be applied in nuclear physics.

The conference was concluded with a meeting of the IT4Innovations Users Council, where Jan Heyda from the University of Chemistry and Technology in Prague was elected the new Chairman of the IT4Innovations Users Council. He replaced Paolo Nicolini from CTU Prague in the position of the Chairman.

Full photo gallery HERE

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WE USED THIS OPPORTUNITY TO ASK JAN HEYDA A FEW QUESTIONS.

Can we ask for a brief reflection of this year's conference?

"This year's number of participants and contributions clearly indicates that the IT4Innovations Users Conference has found a firm place in the calendar of members of the computing and supercomputer community. The conference is unique for the wide spectrum of presented topics. In my opinion, it is a great opportunity to meet with experts in different fields of study in one place and become familiar with their current research work. It is these meetings, which help us understand the needs of other computing laboratories and present a perfect place for gaining a certain scientific bird's eye view."

It is the first time the conference has been held as a two-day event. Do you personally view this change positively?

"The two-day format of the conference had already been proposed by the Executive Board with a slightly different programme earlier. Although two-day conference participation is more challenging in terms of organisation for university-based attendees during an academic year, this format undoubtly has its uncontested advantages. In particular, it offers more time for the informal part, discussions, and poster presentations of professionally younger colleagues. I am personally happy for this, in my opion, quite positive change."

During the conference, the IT4Innovations Users Council took place as well. Can you briefly summarise the results of this meeting?

"An important feature was the election of the new Executive Board, i.e the body representing the IT4Innovations Users' Council. Paolo Nicolini, the first Chairman, managed to set up a functional Executive Board consisting of members across research institutions in the Czech Republic. I would like to use the opportunity to thank Paolo for having done such a great job and wish him a successful scientific career.

The newly filled-in Executive Board will collect the suggestions of users. With respect to the ever growing excess of demand over the allocated computing time, we continue to find other ways to use it as fully and efficiently as possible. A number of users certainly appreaciated being introduced to the project proposal evaluation process, which is transparent, unbiased, and naturally takes into account the publications produced with the support of the IT4I infrastructure."

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LOOKING BACK AT THE LATEST SUPERCOMPUTING CONFERENCE

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Supercomputing Conference – SC19

At the end of November, IT4Innovations traditionally participated at the world's most prestigious conference focused on HPC – Supercomputing Conference (SC19). It was already its 31st edition entitled "HPC is Now" and took place in Denver, USA, with almost 14,000 visitors.

The six-day conference programme, which included lectures, workshops, discussion forums, and a poster section, was made up of contributions from across the HPC research domains by 1,150 speakers. The poster section also featured a poster by Vojtěch Címa, Jakub Beránek, and Stanislav Böhm from IT4Innovations entitled ESTEE: A Simulation Toolkit for Distributed Workflow Execution. Jakub Beránek's article 'Network-Accelerated Non-Contiguous Memory Transfers' featured in the Network and Memory Specialization section. The presentation of the HyperLoom project poster by ADAS Laboratory from 2017 was included in the SC History exhibition from 1988 to 2019, which was a really nice surprise.

The conference's inherent part is the SC Exhibit, with the latest one bringing together under one roof 370 exhibitors including hardware producers, universities, and research organizations from all over the world. For the seventh time in a row, IT4Innovations National Supercomputing Center was one of them. For four days, the presentation of the infrastructure and research of the IT4Innovations, as well as many meetings, took place at its exhibition booth. The LEXIS project coordinated by IT4Innovations was also presented there. For the entire duration of the conference, our booth hosted more than 350 visitors.

"It was great to see such high interest of visitors in the presentation of our research activities as well as infrastructure at the exhibition booth. Visitors were primarily interested in the new petascale system, which is to be installed at IT4Innovations in 2020. Moreover, I consider the LEXIS project presentation, which took place at the booth at the same time and wasreserved half of the presentation area, to be highly valuable as well. The visitors were literally drawn in by this project. This was caused to considerable extent by the neighbouring booth dedicated to the European exascale projects," says Vít Vondrák, IT4Innovations Managing Director.

SC19 PRESENTATIONS AND POSTERS

For posters and presentations from SC19, see HERE. For videos, see HERE and images HERE.

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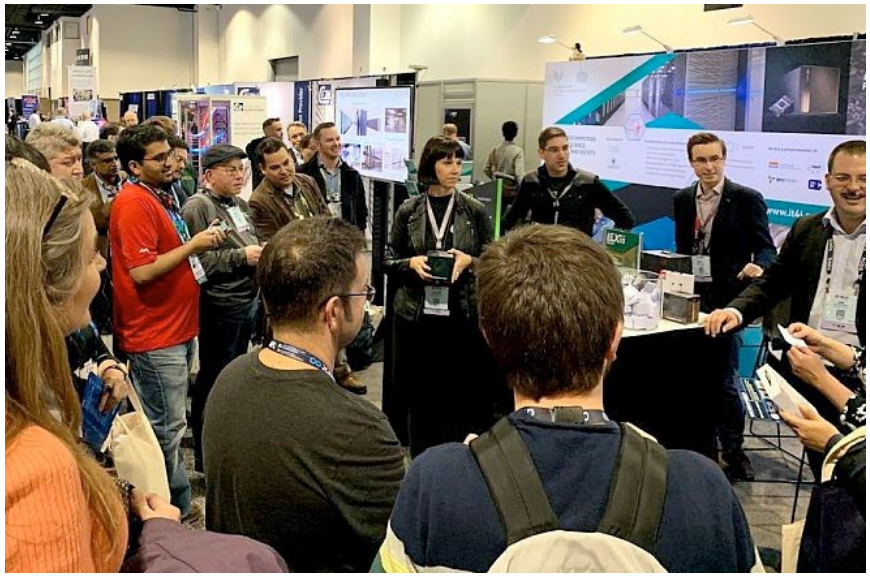

Conference – SC19

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China is reinforcing its top position in the number of supercomputers in the TOP500 list, the most powerful ones are still in the USA

The TOP500 list of the world's most powerful supercomputers is updated twice a year – at the ISC conference in June and the SC conference in November. The 54th edition of the TOP500 showed that China and USA maintain their dominant positions, albeit in different categories. The USA still posseses of the world's most powerful supercomputers – the top position is occupied by the Summit supercomputer installed at the Oak Ridge National Laboratory with a theoretical peak performance of 200 PFlop/s and the Sierra supercomputer installed at the Lawrence Livermore National Laboratory with a theoretical peak performance of 125 PFlop/s. China dominates the list in the number of supercomputers, which is currently 227. The aggregate supercomputing performance of the 500 supercomputers amounts to 1.65 exaFlop/s. The major suppliers include Lenovo (174), Sugon (71), Inspur (65), Cray (36), and HPE with 35 installed systems.

Since 2015, the TOP500 list has also been featuring the only representative from the Czech Republic, Salomon, operated by IT4Innovations. When entering the list, it was wonderfully at 40th place, whereas now it is ranked 375th – in the last six months alone its position dropped by 93 from the 282nd place. However, the situation is about to change this year. The new petascale EURO_IT4I system will be installed at IT4Innovations with the ambition to rank in the European's top 10 and the world's top 40.

For more information, see HERE

TOP500 List – top 10 of the world's most powerful supercomputers

Name / Country / Theoretical peak performance		
Summit	USA	200 PFlop/s
Siera	USA	125,8 PFlop/s
Sunway TaihuLight	China	125,4 PFlop/s
Tianhe-2A	China	100 PFlop/s
Frontera	USA	100 PFlop/s
Piz Daint	Switzerland	27 PFlop/s
Trinity	USA	41 PFlop/s
AI Bridging Cloud Infrastructure	Japan	32 PFlop/s
SuperMUC-NG	Germany	26 PFlop/s
Lassen	USA	18 PFlop/s

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REVIEW OF 2019'S EVENTS AND ACTIVITIES

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In 2019, we welcomed more than 2,190 visitors. We organized 68 excursions, with most of them being around our infrastructure, for both specialists and the general public. We also took a very active role in organising specialised courses with a total of 249 participants. Additionally, we held the traditional IT4Innovations Users Conference, as well as the international HPCSE 2019 conference with the participation of nearly 100 visitors.

We also actively participated as usual at the prestigious international ISC 2019 conference in Frankfurt, Germany, as well as at the Supercomputing Conference (SC19) in Denver, USA. For the first time, we attended the LINUX Days held in Prague.

The general public had the opportunity to learn more about IT4Innovations at the Science Fair in Prague, at the Tour around Projects exhibition in Ostrava, at the Art&Science festival at VSB-TUO, through our coordination of the Superheroes 4 Science Visegrad outreach project, and at the NATO Days – the biggest event of the Moravian-Silesian Region. Moreover, more than 700 visitors came to see our centre on Researcher's Night.

REVIEW OF COURSES ORGANIZED IN 2019

- 14th and 15th January 2019: Developing efficient HPC applications for the latest CPU architectures with C++ and Fortran (PTC course)
- 26th March 2019: Parallel visualization of scientific data using Blender (PTC course)
- 4th April 2019: Parallel visualization of scientific data using Blender
- 24th and 25th April 2019: Data science with R and Python (PTC course)
- 11th June 2019: Fundamentals of Deep Learning for Computer Vision (PTC course)
- 3rd September 2019: Fundamentals of Deep Learning for Computer Vision (IT4I training)
- 16th and 17th October 2019: Productivity tools for High Performance Computing (PTC course)
- 11th and 12th November 2019: Get Started with Intel and NVIDIA Artificial Intelligence Technologies (PTC course)

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