

NEWSLETTER Q2/2019

VSB TECHNICAL
UNIVERSITY
OF OSTRAVA

IT4INNOVATIONS
NATIONAL SUPERCOMPUTING
CENTER

Our supercomputers are about to rank among the ten most powerful supercomputers in Europe	5
IT4Innovations succeeded in the pan-European competition to host the EuroHPC petascale supercomputing system.	
How to obtain access to NVIDIA DGX-2	9
The NVIDIA DGX-2, a system primarily designated for artificial intelligence computations was officially launched in March this year. How can you obtain access to this new system?	
Within the e-INFRA CZ project, we have joined two other research infrastructures	11
Together with CESNET and CERIT-SC, we have submitted a joint project aimed at building a modernized national large research e-INFRA CZ e-infrastructure.	
We organized the HPCSE conference presenting the cutting edge of supercomputing and other fields	13
The HPCSE conference provided an opportunity for about 100 students and experts to share their experience in the field of supercomputing technology. We are bringing you an interview with one of the speakers.	
Evaluation of the 16 th Open Access Grant Competition	17
We distributed 73 million core hours across 54 successful projects at the beginning of June 2019. We introduce selected projects, which were awarded our computational resources.	
We have become members of the prestigious organizations Big Data Value Association and EUDAT Collaborative Data Infrastructure	23
We have joined two important associations.	
We are part of a centre focused on applied research in diagnostics and treatment of rare and genetic diseases	25
Since March this year, we have been part of the research consortium - the PerMed National Centre of Competence.	
Energy efficient applications to reduce energy consumption of supercomputers	27
The READEX project aimed at reducing energy consumption of supercomputers has been successfully completed. Using the newly developed READEX tools, maximum energy saving as high as 34 % has been achieved during tuning of production applications.	
Successful completion of the ANTAREX project	29
We have also successfully defended before the representatives of the European Commission the results of the ANTAREX project where we primarily participated in development of the intelligent navigation system.	
Where you might have seen us	31
We were visited by the Czech Prime Minister	38

INVITATIONS

FUNDAMENTALS OF DEEP LEARNING FOR COMPUTER VISION COURSE

**3rd September 2019,
IT4Innovations**

The Fundamentals of Deep Learning for Computer Vision course is designated for students, academics, and researchers who would like to learn to train and use neural networks for solving real problems. The course will take place on 3rd September 2019, and you may register until the course is full by 26th August 2019.

For more information, see www.it4i.cz

INVITATION TO THE 3RD IT4INNOVATIONS USERS CONFERENCE

**5th November 2019,
IT4Innovations**

We are happy to invite all IT4Innovations users to the 3rd IT4Innovations Users Conference, which will be held on 5th November 2019 at IT4Innovations. The participating users are welcome to contribute to the conference programme with their presentation or research poster within the registration of contributions by 20th August 2019.

For more information, see www.it4i.cz

COME AND VISIT US IN SEPTEMBER

**5th September 2019 –
Art&Science**

A day-long event for the general public, crowned with a concert by Monkey Business will take place on the campus of VSB – Technical University of Ostrava. We are looking forward to meeting you at our booth dedicated to the Superheroes for Science.

**21st to 22nd September – NATO
Days**

You can meet us at our booth at the NATO Days at Mošnov airport already for the third time.

**27th September 2019 –
Researchers' Night**

At the building of IT4Innovations, interesting presentations and guided tours around our infrastructure will take place within the event of Researchers' Night.

Follow us on Facebook



IN BRIEF

IT4INNOVATIONS IN MEDIA

Read an article about new petascale supercomputer to boost research in Central and Eastern Europe published in Science Business Magazine.

For more information, see sciencebusiness.net

REVIEW 2018 PUBLICATION

The review of the most important events, significant achievements, results, and projects in 2018 can be found in our new Review 2018 publication.

For more information, see www.it4i.cz

THE LOW-POWER WAN SEMINAR SUPPORTED BY THE H2020 TETRAMAX PROJECT WAS ORGANIZED

On 24th – 25th April 2019, the Low-Power WAN seminar, where Professor Miroslav Vozňák introduced the [TETRAMAX](http://www.tetramax.eu) project and low-power sensor networks to the participating company representatives, was held.

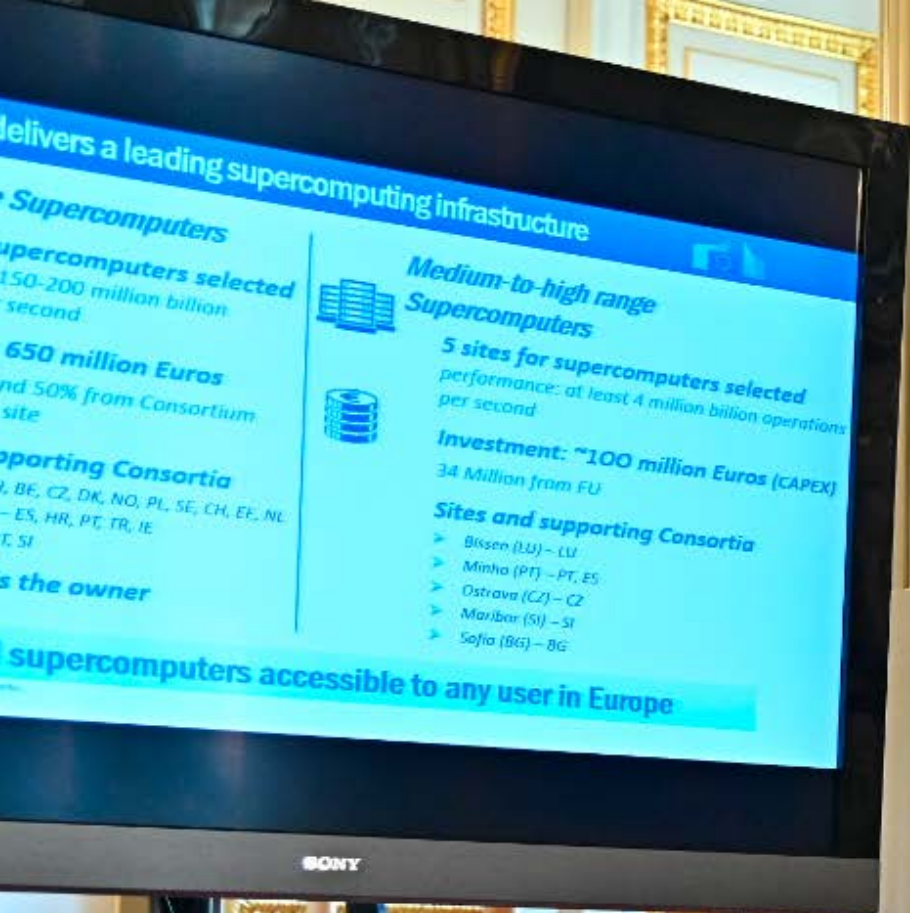
For more information, see www.tetramax.eu

SUPECOMPUTING IN SCIENCE AND ENGINEERING 2017-18 PROCEEDINGS

The publication containing 51 selected contributions from the users of our supercomputing systems for the last two years can be found online.

For more information, see www.it4i.cz





EUROHPC PETASCALE
SUPERCOMPUTING SYSTEM



Our supercomputers are about to rank among the ten most powerful supercomputers in Europe



IT4Innovations has succeeded in the pan-European competition to host the EuroHPC petascale supercomputing system, which will be built in the EU within the joint technological EuroHPC initiative. Of a total of 5 submitted proposals, the Czech project titled IT4Innovations Center for European Science and Industry was awarded 95 of a maximum of 100 points by the evaluation committee, thus winning 1st place. The participants in the competition to host the EuroHPC petascale supercomputing system also included Luxembourg, Portugal, Slovenia, and Bulgaria. Ultimately all 5 submitted proposals will probably be supported, taking into account their quality.

Winning the hosting of the petascale supercomputer, however, was not the only successful project achieved by IT4Innovations as well as the Czech Republic. In 2020, the **LUMI** (*Large Unified Modern Infrastructure*) consortium formed by Finland as the Coordinator together with Belgium, the Czech Republic, Denmark, Estonia, the Netherlands, Norway, Poland, Sweden, and Switzerland is to procure the EuroHPC pre-exascale supercomputer, the installation of which will take place in Kajaani, Finland, and will rank among the most powerful supercomputers worldwide.

The Vice-President of the European Commission for Single Digital Market, Andrus Ansip, in relation to placing the new European supercomputers stated, *“These new centres will allow scientists and researchers access to world-class state-of-the-art supercomputers. They will allow data to be processed directly in the EU rather than in supercomputing centres outside its territory. For Europe it marks the decisive step towards reaching a brand new level of computing power. It shall help us make more significant progress in developing future technologies such as the Internet of Things, artificial intelligence, robotics, and data analysis.”*

With its parameters, the new supercomputer will rank among the most powerful supercomputers in Europe. It will be installed in the upcoming year, and it can be expected to rank among the 50 most powerful supercomputers in the world. In Europe, it will take its position in the top ten. The system is designed so as to fully cover the demands of users in solving complex scientific as well as industrial problems including standard numerical simulations and advanced data analysis or use of artificial intelligence.

Official ceremony dedicated to the placement of the EuroHPC supercomputer at IT4Innovations, Prague, 13th June 2019, source: MŠMT

The investment costs related to procurement of this system are expected to reach a total of EUR 15 mil., with 35 % of the costs, i.e. EUR 5.25 mil. being covered by the European Commission. The remaining costs will be covered by the resources of the European structural and investment funds from the Operational Programme Research, Development, and Education (OP RDE). The system is expected to be procured in 2020, with its operating costs in 2020 to 2025 being EUR 14 mil.

The official announcement about the placement of the EuroHPC supercomputer at IT4Innovations National Supercomputing Center was made on **13th June 2019** at the Ministry of Education, Youth and Sports on the occasion of the visit of Khalil Rouhana, the Deputy Director-General of the European Commission for Communication networks, Content, and Technology, in the Czech Republic.

"We are honoured that the IT4Innovations supercomputers will play such an important role in implementing key scientific experiments and boost industrial sectors in applying scientific knowledge in practice," Vít Vondrák summarizes the achievements of IT4Innovations.

In the upcoming months, the joint EuroHPC undertaking will sign agreements with the consortia. The supercomputers are planned to be put into operation and made available to European users from academia, industry, and the public sector in the second half of 2020. All supercomputers will be connected to the high-speed pan-European GEANT along with the existing supercomputers, which are part of the pan-European PRACE research infrastructure.

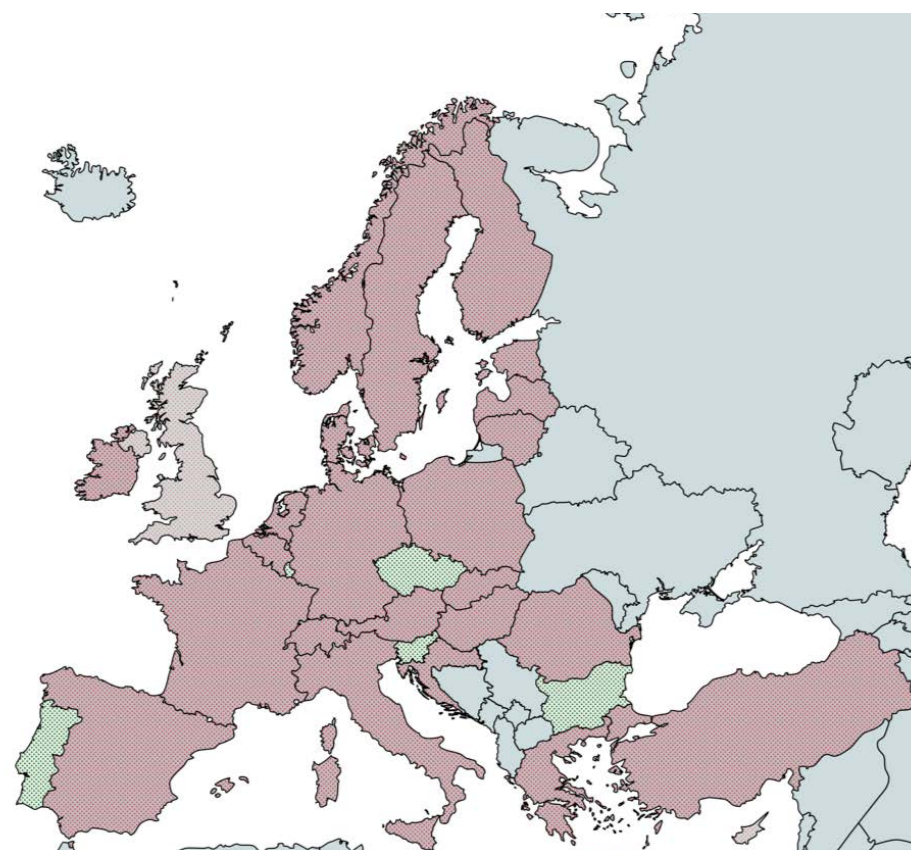
The new supercomputer to be located at IT4Innovations shall reach a theoretical peak performance of 13.6 PFlop/s, which corresponds to 13.6 quadrillion floating point operations per second.

The supercomputer will consist of 6 main parts:

1. a universal part for standard numerical simulations, which will be computed by approximately 600 computer servers with a theoretical peak performance of 2.23 PFlop/s,
2. an accelerated part with 70 servers, with each of them being equipped with 8 GPU accelerators providing a performance of 6.3 PFlop/s for standard HPC simulations and 100 to 150 PFlop/s for artificial intelligence computations,
3. a part designated for large dataset processing that will provide shared memory of as high as 24 TB, and a performance of 74 TFlop/s,
4. 36 servers with a performance of 131 TFlop/s will be reserved for providing cloud services,
5. a high-speed network to connect all parts as well as individual servers at a speed of up to 100 Gb/s,
6. data storages that will provide space for up to 7.5 PB of user data and will also include high-speed data storage with a speed of 1 TB/s for simulations as well as computations in the fields of advanced data analysis and artificial intelligence.

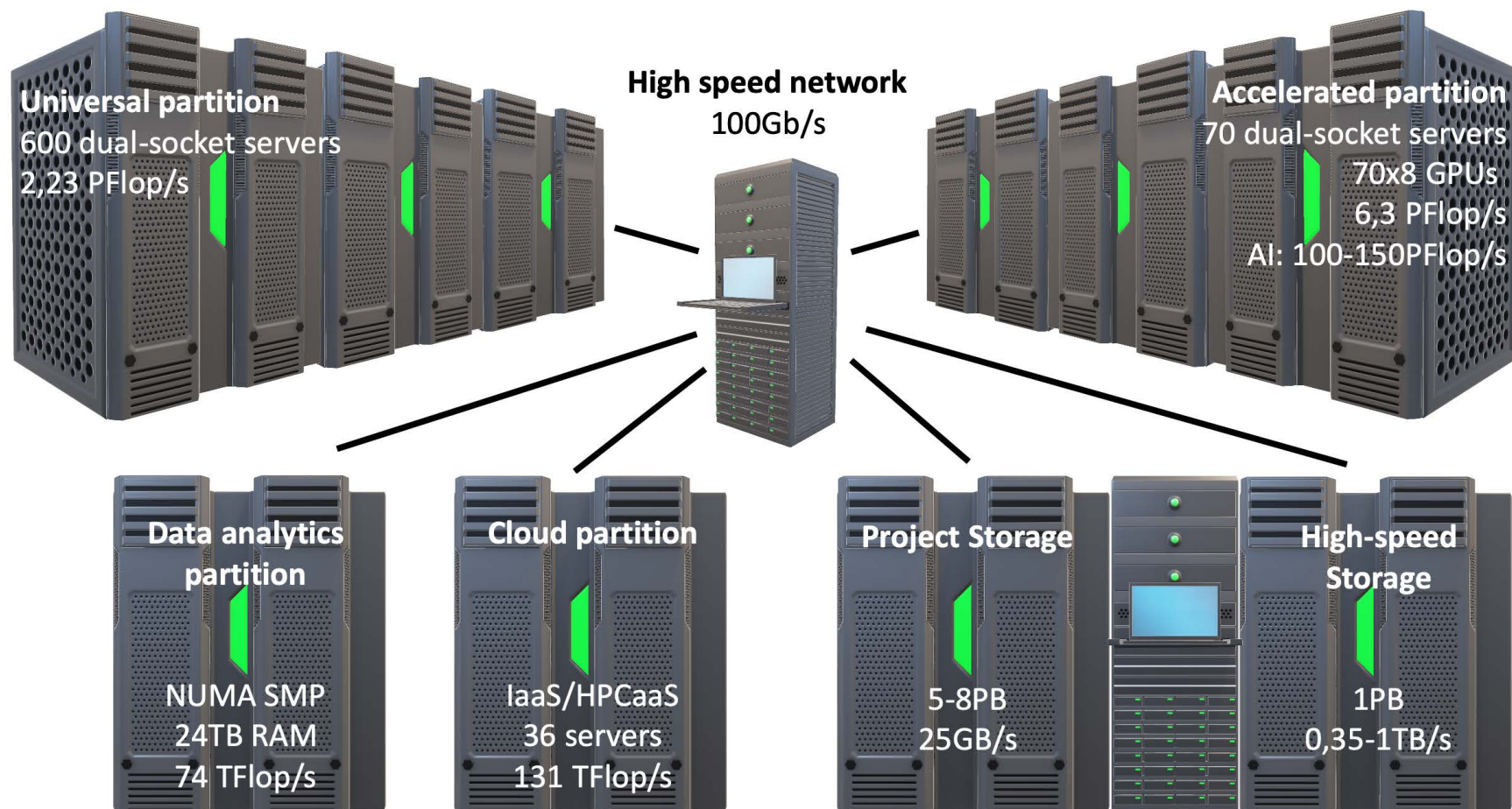
EuroHPC countries/petascale candidates

- Participating country
- Observer country
- Petascale hosting entity candidate





EuroHPC
Joint Undertaking



Video about the placement of the EuroHPC supercomputer at IT4Innovations: [youtube.com](https://www.youtube.com/watch?v=...)



ACCESS TO NVIDIA DGX-2



How to obtain access to NVIDIA DGX-2

The NVIDIA DGX-2, system primarily designated for artificial intelligence computations was officially launched in March this year. In order to get access to the system, you have to be active users of our supercomputing infrastructure and have the computational resources of our systems allocated.

You can apply for the computational resources either within our Open Access Grant Competitions, which are announced three times a year, or by submitting an application through the Director's Discretion scheme anytime. It is an irregular allocation of computational resources, which can be obtained by users from non-commercial spheres in case the Open Access Grant Competition cannot be used.

In the case of submitting a brand new application within the Open Access Grant Competition, you can already specify that you are interested in the GPU (Graphic Processing Unit) compute nodes as well as which supercomputer you would like to use.

Once you are awarded the IT4Innovations computational resources, you can request access to NVIDIA DGX-2 by writing an e-mail to support@it4i.cz explaining the amount of computational resources of NVIDIA DGX-2 you need and primarily their purpose. The decision to allow access and award the computational resources of the system is made by the IT4Innovations management, who inform the user immediately.

On NVIDIA DGX-2, tasks are run practically identically as on the Anselm and Salomon clusters. This solution is unique and has been developed by our colleagues from the Supercomputing Services department. The system is accessed through the scheduler from Salomon login nodes, and the scheduler can be accessed by loading the DGX-2 module.



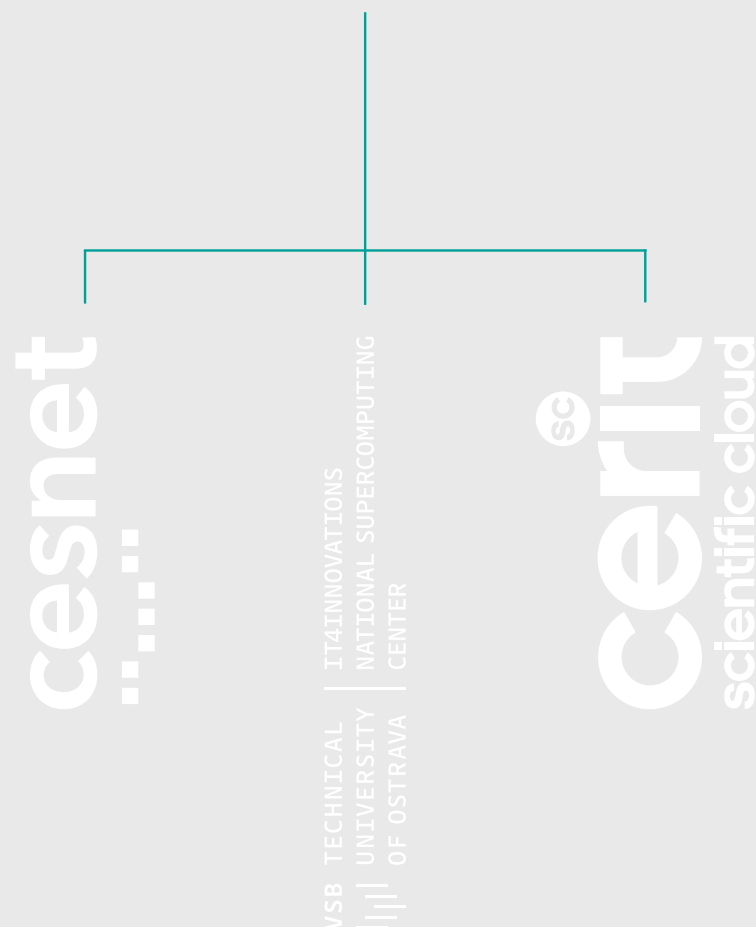
Video about the NVIDIA DGX-2 system installation in our data room: [youtube.com](https://www.youtube.com/watch?v=...)



E-INFRA RESEARCH INFRASTRUCTURE



e-INFRA CZ



Within the e-INFRA CZ project, we have joined two other research infrastructures

Together with CESNET and CERIT-SC, we have submitted a joint project aimed at building a modernized national large research e-INFRA CZ e-infrastructure. Prior the submission of the project, a partner agreement where we have undertaken to participate in cooperation based on operating, developing, and providing a full portfolio of services of the e-INFRA CZ infrastrure was concluded.

e-INFRA CZ connects all three existing bodies of the national e-infrastructure:

- CESNET
- CERIT-SC operated by Masaryk University
- IT4Innovations National Supercomputing Center operated by VSB – Technical University of Ostrava

All bodies were incorporated in the ESFRI Roadmap already in 2010 with the e-INFRA CZ project being an evolutionary step towards its closer integration.

e-INFRA CZ is a fully transparent environment providing complex capacity and resources for transfer, storage, and processing of scientific data for entities involved in research, development, and innovation across sectors. It has created a communication, information, storage, and computing platform for research, development, and innovation on the national as well as international level, and provides a broad and complex portfolio of ICT services essential for modern research, development, and innovation.

“One of the main contributions of our participation in the joint e-INFRA CZ project can be considered the improvement of accessibility of our supercomputing technology and services for a wider scientific community in the Czech Republic,” says Vít Vondrák, the Managing Director of IT4Innovations National Supercomputing Center.

The main parts of e-INFRA CZ include:

- High-performance national communication infrastructure
- National grid and cloud infrastructure
- The most powerful and modern supercomputing systems in the Czech Republic
- High-capacity data storages

Other tools and services such as access management of ICT resources, tools supporting distant cooperation, or tools for securing safe communication and data protection also present an inseparable part and added value of the infrastructure.

The infrastructure significantly boosts new drug design, personalized medicine, materials research and nanotechnology development, natural disaster prediction, research in the field of security and environmental protection, development of new energy sources and intelligent transport systems, and implementation of Smart City and Industry 4.0 concepts.

For more information, see www.it4i.cz





HPCSE 2019 CONFERENCE

We organized the HPCSE conference presenting the cutting edge of supercomputing and other fields

In May 2019, we organized the 4th High Performance Computing in Science and Engineering (HPCSE) conference at Hotel Soláň in the Beskydy Mountains. Nearly 100 experts and students from different parts of the world had the opportunity to exchange experience in the field of HPC technologies and other scientific domains that use these technologies or benefit from them.

During the four consecutive days, more than thirty presentations mapping the latest research results were heard. The participants thus had a unique opportunity to exchange experience and information in applied mathematics, numerical methods, high performance computing, data analysis, and scientific data visualization.

The conference featured renowned speakers from both the Czech Republic and abroad.

Jakub Kurzak from the University of Tennessee in the United States presented the SLATE (Software for Linear Algebra Targeting Exascale) software for exascale supercomputers of the United States Department of Energy, the development of which is led by Jack Dongarra, the doyen of HPC and the supercomputing world. The topic of exascale and software development is also the domain of Dominik Göldeke from the University of Stuttgart in Germany. Furthermore, Garth Wells from the University of Cambridge spoke about supercomputing for solution of engineering



problems, namely turbo machines. Andrea Bartolini from the University of Bologna in Italy presented his paper summarizing several years of research focused on innovative technologies for future green and intelligent supercomputers. Lubomír Říha from IT4Innovations introduced the participants to a new approach to loading of datasets generated by unstructured meshes for which IT4Innovations develops massively parallel solvers. .

"I personally enjoyed the HPCSE conference as it was very pleasant and fruitful. I established several new relations, and what is more, a few ideas occurred to me. I would like to mention some aspects of the conference. At first, I thought that the contributions would be particularly aimed at high performance computing. To my surprise, they covered a wide spectrum of interesting areas ranging from basic research to industrial design and movie rendering. The technical quality was high, and I found the brief introduction of poster authors something I would appreciate at other conferences as well, particularly valuable," said Ben T. Cox, the Head of the Biomedical Ultrasound Group based at University College London, which is involved in numerical simulations of acoustic waves propagation used in seismology and medicine.

INTERVIEW WITH GÜNTHER OF FROM GRAZ UNIVERSITY OF TECHNOLOGY

At the HPCSE conference, we asked Günther Of, one of the invited speakers, a few questions. Günther Of is established at Graz University of Technology (TU Graz). Together with our colleagues from the BEM4I team (part of the Parallel Algorithms Research Lab) he is involved in implementing a three-year Czech-Austrian project titled 'A parallel space-time boundary method for the heat equation', funded by Fonds zur Förderung der wissenschaftlichen Forschung (the Austrian agency for science) and the Grant Agency of the Czech Republic. Work on the project started at the beginning of this year.



Do you remember what the most exciting thing about mathematics and the boundary element method, in particular, was?

"At secondary school you practically have no idea what mathematics is about. However, I somehow liked it and decided to study it. When it comes to the boundary element method, I stumbled upon it by accident. Olaf Steinbach, who later became my diploma and dissertation supervisor, led a seminar focused on the fast boundary element methods. At that time this topic presented a challenge. One other student and I were the only registered ones for the seminar. Olaf organized a workshop with some of the experts in the field where we presented our seminar work. Therefore, we later focused on this topic in my diploma thesis."

It was your first time participating at the HPCSE conference we organize. You presented the research within the Czech-Austrian project titled 'A parallel space-time boundary method for the heat equation'. Can you please briefly introduce your research to the readers who were not present at the conference?

"The objective of this project is to calculate time-dependent temperature distribution in a building using efficient numerical simulation. Conventional approaches which allow calculation of changes in small time steps are not able to fully use the potential of the latest supercomputers. For the overall calculation we use a space-time method, which allows parallelization in time. In doing so, we can distribute the calculation across more processors and obtain the result in a much shorter time. However, there are certainly some problems associated with the efficiency of numerical processing and parallelization of this method, which we aim to overcome within our joint project."

How was your cooperation with the Czech team established?

"I have known the colleagues from Ostrava – Zdeněk Dostál, Dalibor Lukáš and others – for a long time. As much as me, they are involved in research focused on domain decomposition methods, and we often meet at conferences. Our mutual contacts have always been supportive and friendly despite



coming up with similar ideas. Thanks to these good relationships, Jan Zapletal managed to get to our institute, Graz University of Technology, to participate in implementing European project Controlled component and assembly-level optimization of industrial devices, which was led by Z. Andjelic, F. Cirak, C. Trinitis, and O. Steinbach. Michal Merta and I met at the Fast BEM and BETI workshop in Ostrava in 2012, where I was invited to lecture. Based on our outstanding relationships, we jointly led a scientific and technological cooperation titled Efficient parallel implementation of boundary element methods in 2017 and 2018. The mobility grant was provided by Austrian agency Österreichischer Austauschdienst (OeAD) and the Ministry of Education, Youth and Sports of the Czech Republic.

Within our successful cooperation, we decided to submit the Czech-Austrian project A parallel space-time boundary element method for the heat equation, and to apply to the Austrian agency for science Fonds zur Förderung der wissenschaftlichen Forschung and the Grant Agency of the Czech Republic for funding. Initially, it was supposed to be an individual project in this field. Nevertheless, we realized that by combining our knowledge in numerical methods analysis and high-performance computing we could create a much more robust design. The fact that we place more emphasis on HPC would eventually lead us to developing a competitive solver."



How did you enjoy the HPCSE 2019 conference and how productive was it for you?

"I really liked the venue of the conference, just the weather was not very favourable. However, it did not prevent us from attending interesting presentations. From time to time, I had the opportunity to meet the colleagues from Ostrava in the past, yet we were rather busy. Therefore, I really appreciated to meet them at the conference and discuss things in more detail."

Was there any other research project that you were particularly interested in presented at the conference?

"Many exciting presentations were heard at the conference. I am mainly involved in the field of numerical analysis and manage to apply parallelization to a certain degree. Yet, I am not an expert in the field. It was highly beneficial for me to get a valuable insight into the HPC field from different perspectives. I was surprised by the quality of the poster section. At most conferences, little attention is paid to these sections. At the HPCSE conference, on the other hand, the participants showed a great interest in the posters."

It was a pleasure speaking with you and wish you great success.

For photos, see the following HPCSE conference website: hpcse.it4i.cz

EVALUATION OF THE 16TH OPEN ACCESS GRANT COMPETITION



In the 16th Open Access Grant Competition (OAGC), the interested candidates applied for more than **127 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 **93 %**. Therefore, the Allocation Committee had to agree to lower the allocations of the evaluated projects. Within this OAGC the interested candidates could also apply for multi-year access (18-, 24-, and 36 months access). We distributed 73 million core hours across 54 successful projects, six being multi-year projects, at the beginning of June 2019.

Almost half of the successful projects (21) fall into material sciences followed by biosciences. Altogether 21 projects were

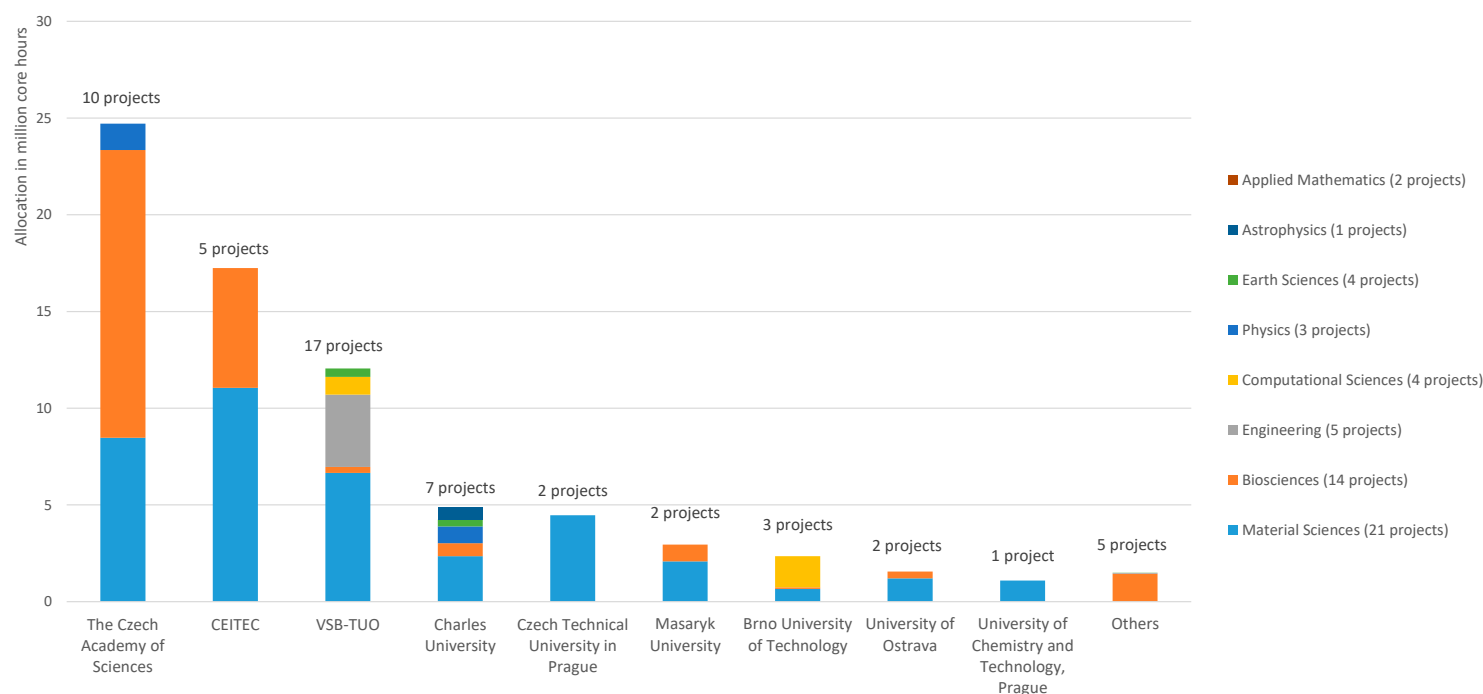
each awarded an allocation of more than 1 million core hours. The investigators of these projects are researchers from 9 different organizations, namely, for example, the Czech Academy of Sciences, CEITEC, IT4Innovations, the Czech Technical University in Prague, and Masaryk University.

In this OAGC, 6 institutes of the Czech Academy of Sciences were awarded computational resources amounting to nearly 25 million core hours (34 % of the total allocated computational resources) for 10 projects. About 17 and 12 million core hours were allocated to the projects of researchers from CEITEC and applicants from VSB – Technical University of Ostrava (mainly from IT4Innovations), respectively.

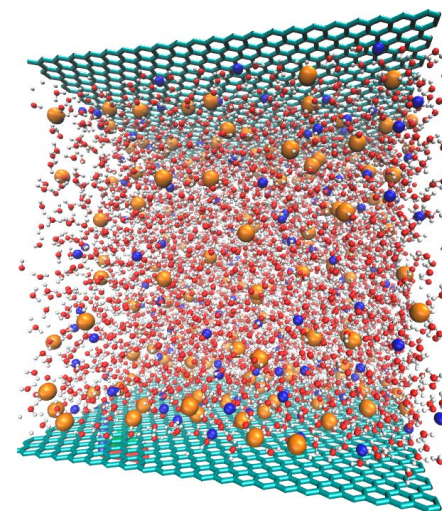
The first three highest allocations were awarded to the projects of our long-term applicants, Prof. Pavel Hobza from the Czech Academy of Sciences (more than 8 million core hours), Prof. Mojmír Šob from CEITEC (more than 7 million core hours), and Prof. Pavel Jungwirth from the Czech Academy of Sciences (more than 5 million core hours).

Besides the organizations shown in the graph, projects from the Czech University of Life Sciences in Prague, Palacký University in Olomouc, Tomas Bata University in Zlín, and the Czech Aerospace Research Centre were also awarded our computational resources.

Allocation of computational resources in the 16th Open Access Grant Competition by research domains and organizations



WE ARE INTRODUCING SELECTED
PROJECTS WHICH WERE AWARDED
OUR COMPUTATIONAL RESOURCES
IN THE 16TH OPEN ACCESS GRANT
COMPETITION



NaCl solution defined by graphene lattice

Dr Barbora Planková
Czech Academy of Sciences

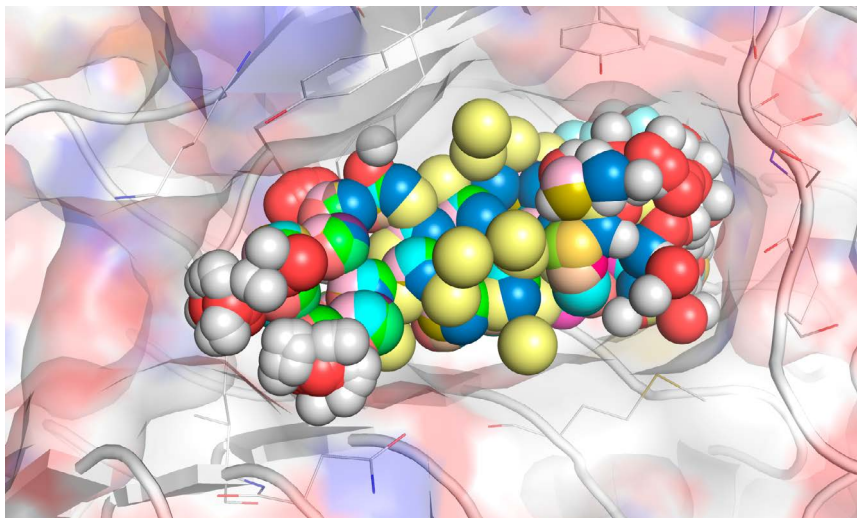
MOLECULAR AND MESOSCOPIC SIMULATIONS OF AQUEOUS SOLUTIONS IN INHOMOGENEOUS ENVIRONMENTS

Barbora Planková from the Institute of Chemical Process Fundamentals of the Czech Academy of Sciences was awarded more than 1 million core hours for molecular and mesoscopic simulations of aqueous solutions in non-homogenous environments. Aqueous solutions are omnipresent in nature, industrial processes, and daily life. Understanding their behavior in inhomogeneous environments (nanopores, self-assembled systems) is important in many key applications such as medicine and environmental protection.

Together with her colleagues, Karel Šindelka and Martin Lísal, Planková will use the supercomputer in three research areas. The first one is graphene-aqueous electrolyte interfaces. Graphene is also called the miracle material of the 21st century. Graphene membranes, for example, could be used in water desalination or its cleaning. First of all, however, it is important to understand the elementary molecular processes, which will be studied by the project author using the supercomputer.

The second research area is focused on ionic surfactants used, for example, in fabric conditioners. Part of the allocated computational resources will be used to study of the behaviour of these active substances and their interaction with soft surfaces – the key aspects of their functionality.

The third research area focuses on solubilisation of small molecules in interpolyelectrolyte complexes, which can influence drug effectiveness and removal of pollutants.



Collage as a result of substance docking in the selected steroid receptor. The balls represent individual atoms of a small chemical substance, and the surrounding is the receptor with an active part where individual aminoacids can be seen.

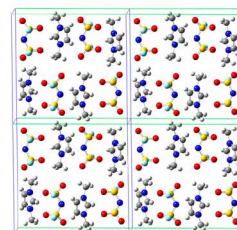
Dr Václav Bazgier
Palacký University in Olomouc

VIRTUAL SCREENING OF HUMAN AND PLANT HORMONES

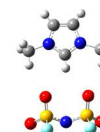
Virtual screening employs supercomputers to discover potentially new chemical compounds, which is a cheaper and less time-consuming approach than their laboratory testing. The computer selects the best performing candidates from a large library of chemical compounds, which are then experimentally tested.

Václav Bazgier from Palacký University in Olomouc was awarded almost half a million core hours for his project titled Virtual screening of human and plant hormones. These hormones play a crucial role in human, animal, and plant life, and are responsible for a number of processes of biological interest. The allocated computational resources will be used in the design of new compounds – hormone-based drugs and fertilizers – by means of molecular docking using data from different databases such as DrugBank and the Human Metabolome Database.

Crystal – Order



Gas – Isolation



Sublimation

**Ab initio
calculations
Molecular dynamics
Statistical
thermodynamics**

Example of crystal and molecular structure of ionic liquid
1,3-dimethylimidazolium bisfluorosulfonylimid

Dr Ctirad Červinka
University of Chemistry and Technology Prague

COHESIVE PROPERTIES OF IONIC LIQUIDS FROM FIRST-PRINCIPLES CALCULATIONS

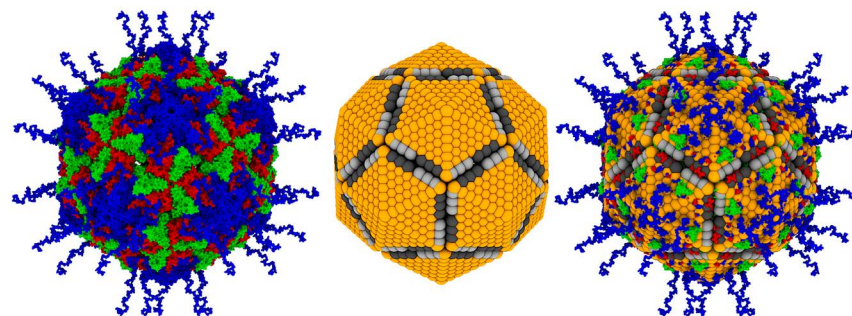
Ctirad Červinka from the University of Chemistry and Technology Prague was awarded more than 1 million core hours for calculations of cohesive properties of ionic liquids. Exhibiting unique properties such as low volatility and boundless structural variability, these ionic liquids possess huge potential for being used in various technologies such as gas capture and smart electrolytes. Broader exploitation of their beneficial characteristics, however, is impeded by their cost as well as insufficient understanding of their physical and chemical properties. Low volatility of ionic liquids, being one of their most valuable properties, is also the principle factor making reliable measurements of their vapor pressures and heat of vaporization extremely difficult. The awarded computational resources will therefore be used to assess the performance of ab initio predictions of sublimation of ionic liquids, aiming to complement or even replace the difficult and hard-to-reproduce vaporization experiments with calculations.

Lukáš Sukeník
CEITEC, Masaryk University

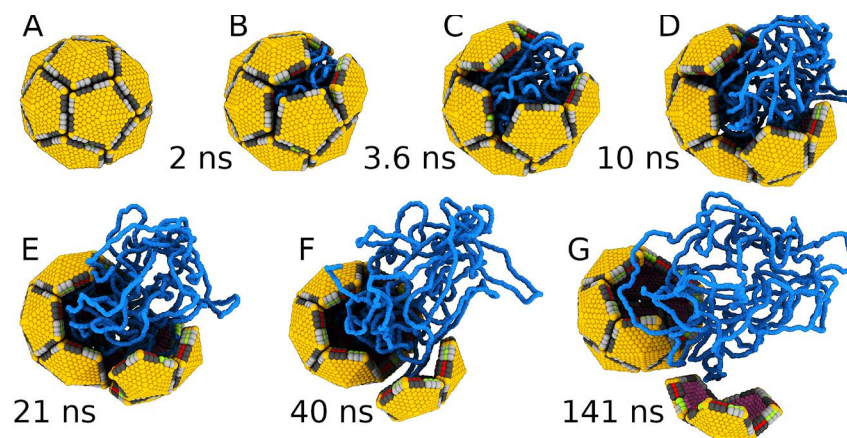
MECHANISM OF GENOME RELEASE OF NON- -ENVELOPED VIRUSES

Many picornaviruses are human pathogens that cause diseases varying from the common cold to life-threatening encephalitis. Currently, there is no picornavirus antiviral drug approved for humans.

Lukáš Sukeník from CEITEC and Masaryk University was awarded more than 4 million core hours to study the mechanism of picornavirus genome release. A cell can be infected once the picornavirus genome is released. These non-enveloped viruses need to transport their genetic material from the protective protein shell (capsid) to host cell cytoplasm. Using the supercomputer and molecular dynamics simulation, Sukeník will study the affects of the capsid properties on genome release. The knowledge obtained will be used for the development of new antiviral therapeutics.



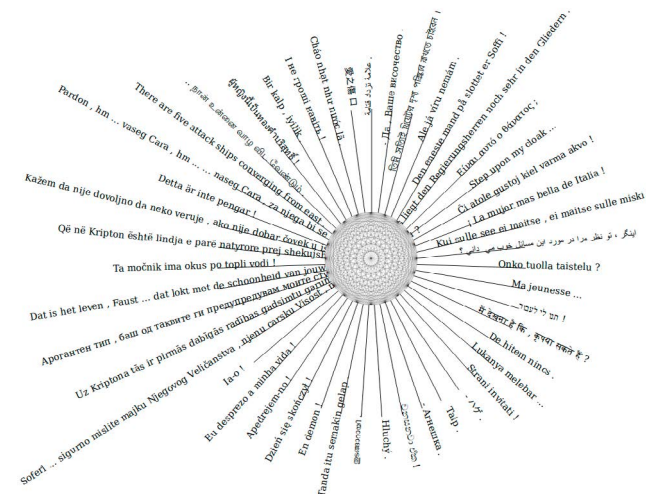
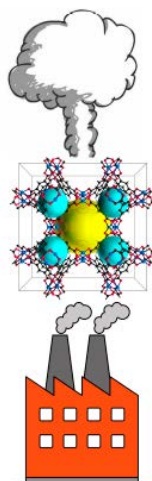
Comparison of the picornavirus atomic structure (left) with the phenomenological model (middle) used in the simulations of the viral genome release mechanism. The virus on the right shows the overlap of both structures as well as equality of the key elements of the structures, i.e. the shape of a regular dodecahedron consisting of 12 individual parts.



Simulation of the mechanism of picornavirus genome release. The selected images show the process mechanism.

- A) Compact capsid before opening.
- B) Initial crack in the protective protein shell (capsid).
- C-E) Gradual release of the viral genome.
- F) A part of the capsid cracking off the whole. The virus genome freely diffusing from the capsid.
- G) The viral genome was successfully released in 141 ns. At this point it attacks the host cell.

Viral genome consists of blue particles. The capsid exterior is yellow, the particles on the edges of different parts of the capsid are grey, red, and green. The red and green particles attract each other and thus model the capsid interactions.



Quantitative analysis of the direct translation quality using the interlingua approach

Dr Pezhman Zarabadi-Poor
CEITEC, Masaryk University

HIGH-THROUGHPUT SCREENING OF METAL-ORGANIC FRAMEWORKS FOR CO₂ SEPARATION FROM A POST-COMBUSTION GAS MIXTURE UNDER HUMID CONDITIONS

Dr. Pezhman Zarabadi-Poor from CEITEC was awarded more than 3 million core hours for identification of the best performing metal-organic frameworks that can separate CO₂ from a post-combustion gas mixture using high-throughput systematic screening.

The main anthropogenic source of CO₂ emission is combustion of fossil fuels. Economic growth and industry development have continually been contributing to its concentration increase in the atmosphere, which leads to global warming of the Earth. One of the most efficient methods to avert this unwanted phenomenon and to maintain industrial development is Carbon Capture Sequestration (CCS). In this regard, metal-organic frameworks (MOFs) are considered attractive solid adsorbents that can efficiently be utilized for carbon capture from one of the main sources of CO₂ emission, i.e. post-combustion gas (average content of CO₂ is 15–16 %).

The supercomputer and the computational resources in the amount of 3.3 million core hours will be used by Zarabadi-Poor to find best performing metal-organic frameworks, which will later be synthesized and experimentally verified in a laboratory. This research is part of the CMPSTORE project funded by the EU Horizon 2020 programme within the Marie Skłodowska-Curie action and co-funded by the South Moravian Region. The project is implemented within the research group of Prof. Radek Marek, and its active participant is Esmail Farajpour Bonab, a student of the Physical Chemistry PhD study programme.

Martin Kolář
Brno University of Technology

DRVOSTEP – OPEN TRANSLATION

DrVostep will investigate the limits of machine translation for hundreds of languages. The first output will be the analysis of translation quality with and without intermediate languages, such as CZ->DE versus CZ->EN->DE. A second result, benefiting the wider European community, will be an open machine translation website like google translate, but unlimited and free by performing client-side computations.

More than 1.5 million core hours were awarded to Martin Kolář from Brno University of Technology to study the quality of translations for hundreds of languages. The current research is generally focused on the development of methods which learn to translate texts between two languages, with no research having been focused on translations among more than 6 languages so far. The objective of Martin Kolář's project is to improve translation quality, to quantify the complexity of languages, and thus find the difference between the quality of direct translation as opposed to translation with an intermediate language. Using our supercomputer, the research team from Brno University of Technology aims to analyse hundreds of languages and develop an open online translator.





WE HAVE BECOME MEMBERS OF THE PRESTIGIOUS
ORGANIZATIONS BIG DATA VALUE ASSOCIATION
AND EUDAT COLLABORATIVE DATA INFRASTRUCTURE

At the end of March 2019 we became a member of the Big Data Value Association, an international non-profit organization. In doing so, we rank among important industrial companies and prestigious research organizations active in the field of big data processing.

The Big Data Value Association (BDVA) has 200 private, public, and academic members from all over Europe. We have joined iconic companies such as IBM, Nokia, Siemens, Philips, SAP, Orange, Atos, and others. The objective of BDVA is to boost Big Data research and innovations.

Big Data and Artificial Intelligence digital transformation aims at developing the pan-European innovation ecosystem to bring the greatest possible contribution to the European economy as well as society, and to reach sustainable European leadership in the above-mentioned areas.

Kateřina Slaninová, an IT4Innovations senior researcher, adds details about the IT4Innovations membership in BDVA: *“Becoming a full member, IT4Innovations can participate in all activities of the organization with full voting rights and the possibility to be elected among the board members. Significant membership advantages also include the possibility to have direct access to negotiations with the European Commission and the membership countries’ representatives. As a result, we will have the opportunity to affect the strategic plan in this field, which I find particularly important.”*

In April, we joined the EUDAT Collaborative Data Infrastructure (CDI). EUDAT CDI is a European e-infrastructure integrating data services and resources to boost research. With its network gathering more than 20 European research organizations and data and computing centres in 14 countries, EUDAT CDI is one of the largest e-infrastructures supporting research in Europe.

The objective of EUDAT CDI is to solve the research data life cycle as a strategic solution of data dissemination in European scientific and research communities. It is implemented through cooperation between service providers and research communities, which operate as part of the common framework for providing information.

“IT4Innovations National Supercomputing Center follows the global trend toward incorporation of HPC technologies and high-speed data services,” says Vít Vondrák, IT4Innovations Managing Director. “Our membership in EUDAT allows us to integrate and provide a wide range of HPC and HPDA services to European research data infrastructures on a deeper level. With our participation in EUDAT CDI, we expect extension of our HPC, HPDA, and data management services for academia as well as industrial enterprises. IT4Innovations will provide its infrastructure and services to EUDAT CDI, and as the H2020 LEXIS project coordinator, IT4Innovations will have an opportunity to use state-of-the-art data management technologies through selected EUDAT CDI services in return,” added Vondrák.

For more information about BDVA, see bdva.eu



For more information about EUDAT CDI, see www.eudat.eu



WE ARE PART OF A CENTRE FOCUSED ON APPLIED RESEARCH
IN DIAGNOSTICS AND TREATMENT OF RARE AND GENETIC DISEASES

IT4Innovations has recently become a member of the research consortium in personalized medicine – the PerMed National Centre of Competence. We have thus joined, for example, the Czech Academy of Sciences, Palacký University in Olomouc, Charles University, University Hospital Brno, St. Anne's University Hospital Brno, and the General University Hospital in Prague, which participate in implementation of this two-year centre of competence funded by the Technology Agency of the Czech Republic (TACR).

The PerMed Centre of Competence is focused on applied research in diagnostics and treatment of rare and genetically conditioned diseases. The objective is to develop personalized diagnostic methods together with substances – candidates for new drugs treating specific groups of patients. The approach is based on the interdisciplinary combination of medicine, chemistry, biology, genetics, and bioinformatics. The entire research is divided into work activities such as validation of right molecular targets, biological chemistry, pre-clinical development, biomarkers identification, and DNA analysis. The PerMed results will be commercialized by selling licences and establishing spin-off companies.

In January 2019, the PerMed Steering Board approved 7 research projects, which were presented at the first work meeting of the centre held at CEITEC in Brno in March 2019. In October 2019, the next meeting of the partners will be held at the Institute of Organic Chemistry and Biochemistry of the CAS.



Meeting of all partners of the PerMed Centre of Competence at CEITEC in March (source: <https://permed.cz/web/>)

PerMed Centre of Competence official website: permed.cz



READEX PROJECT



In December last year, the international READEX (Runtime Exploitation of Application Dynamism for Energy-efficient eXascale computing) project funded by the Horizon 2020 programme was successfully completed. The objective of the project was to reduce energy consumption of supercomputers, which is one of the key problems in building exascale supercomputers.

The main idea of the project is based on the fact that different parts of a parallel application have different demands on hardware resources, and if the resources available are not fully utilized in a given time, these resources or their performance can be disabled or lowered, respectively, with no or limited effect on the application runtime.

One example is the part of an application which is memory bound and whose performance depends only on the speed of the data transfer from the memory to the processor without the computing performance being affected. In this case it is possible to lower the frequency of the processor part (core part) and maintain the maximum frequency of the particular processor part (uncore part) which provides data transfer from the memory. Lowering the frequency of the compute cores, we are able to achieve energy saving. Another possible source of energy savings can be made by completely turning off a certain number of compute cores. One example of a memory bound application is multiplication of a matrix and a vector.

On the contrary, if another part of an application performs multiplication of two matrices, it is part of a code whose performance depends primarily on the

performance of the compute cores and significantly less on the speed of data transfer from the memory (i.e. compute bound parts of an application). In this case, we are able to achieve energy saving by setting a lower frequency for the uncore part of the processor.

The implementation team coordinated by Dresden University of Technology, which consisted of IT4Innovations, the Technical University of Munich, the Norwegian University of Science and Technology (NTNU), the National University of Ireland (NUI Galway), the German GNS mbH (Gesellschaft für Numerische Simulation mbH) company, and Intel, developed a set of tools, which performs the following:

1. Application analysis aimed at identifying the parts of the code with different characteristics,
2. Finding an optimal system setting for the above-mentioned parts,
3. A runtime system, which dynamically tunes an optimal system setting for different parts of the code during the application runtime.

During tuning of production applications using the READEX tools, maximum energy savings of up to 34 % were achieved. Average energy saving amounted to 16.5 %. As a project participant, IT4Innovations was responsible for analysis of the parallel application dynamic tuning potential and the real contribution achieved using the developed tools. With this objective, the MERIC library designated for analysis of possible approaches created within the READEX project was developed. The MERIC library is under continuous development after the completion of the project within other national as well as international projects.

ENERGY EFFICIENT APPLICATIONS TO REDUCE ENERGY CONSUMPTION OF SUPERCOMPUTERS



SUCCESSFUL COMPLETION OF THE ANTAREX PROJECT



Excursion of the participants of the two-day
ANTAREX school at IT4Innovations, October 2018

At the end of January 2019, we successfully defended before the representatives of the European Commission the results of the ANTAREX project in Luxembourg. The objective of the project was to design more energy-efficient running of applications on future heterogenous HPC systems using a domain specific language, auto-adaptive methods, and monitoring.

Our colleagues from the Advanced Data Analysis and Simulation laboratory primarily participated in this project by developing an intelligent navigation system in cooperation with the company Sygic, who are based in Slovakia. Applying the developed algorithms and computing performance of the supercomputer, this navigation system allows efficient distribution of the traffic flow in cities so as to prevent traffic jams or reduce the time spent in them and to keep the traffic balanced and flowing. The pilot system has been able to serve tens of thousands of cars at the same time so far with the objective to reduce the total travel time for all drivers.



Our team with its intelligent navigation system was nominated for the Innovation Radar Prize by the European Committee. This initiative annually identifies European innovators and innovations which are supported by European projects. Based on the voting of the European public, the developed system eventually made it to the finals and was also presented to the community of experts at the ICT 2018 conference in Vienna.

The ANTAREX project was funded by the European Union Framework Programme for Research and Innovation – H2020.



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Joint Undertaking

EuroHPC Summit Week

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EUROHPC SUMMIT WEEK

Within the **EuroHPC Summit Week**, which was held this year in Poznań, Poland, on 13th to 17th May, lectures, workshops, discussions, and presentations of trends in HPC took place. Concurrently with this event, a series of scientific and industrial presentations under the patronage of PRACE - **PRACEdays19** was organized, with four awards being officially announced at its final meeting.

The PRACEdays19 Best Poster Award was won by our colleague Martin Golasowski for his contribution Distributed Environment for Traffic Simulations.



Martin Golasowski with his Best Poster Award at the PRACEdays19 conference (source: PRACE)



Presentation of the LEXIS project at the poster section of the conference





Panel discussion on the future of scientific and industrial computations in Europe



PRACE-6IP KICK-OFF MEETING IN BRATISLAVA

In May this year, the 6th consecutive PRACE
(Partnership for Advanced Computing in Europe)
implementation phase was officially launched by the
kick-off meeting of the project partners in Bratislava,
Slovakia, where individual work groups had the
opportunity to plan their activities for further
successful implementation of the project phase.
We have been a member of PRACE since 2011.

Our colleagues at the official kick-off meeting of
PRACE-6IP in Bratislava, Slovakia (source: PRACE)



JOSEPH FOURIER PRIZE 2019

On Monday 27th May, the **Joseph Fourier Prize Committee** held a session at our centre. The objective of the competition is to award the best students, who significantly contribute by their research work to computer science and information technology fields focused on design and utilization of computer algorithms and methods, simulation and modelling, and

big data processing. This year participants included our colleagues Martin Mrovec and Ondřej Meca.

The official announcement took place on 26th June at the National Museum in Prague. A special IT4Innovations National Supercomputing Center prize – i.e. 50,000 core hours of the Anselm supercomputer – was awarded to Ladislav Maršík from Charles University. In his work, he focuses on the similarity of music compositions based on the harmony.

For more information, see atos.net



Joseph Fourier Prize committee



Winner of the IT4Innovations Special Prize



Ondřej Meca



SCIENCE FAIR

In the first week of June, we participated at the **Science Fair in Prague** organized by the Czech Academy of Sciences, which welcomed 30,000 people this year. The fair featured the cutting edge and attractions of science, new technologies, and innovations at more than 100 expositions of the Czech Academy of Sciences, universities, and innovation companies. At our booth, IT4Innovations and the Superheroes 4 Science, a project presenting supercomputers to children by means of comic strips, were presented.



INTERNATIONAL SUPERCOMPUTING CONFERENCE

In Frankfurt, Germany, in June, the **International Supercomputing Conference (ISC)** welcoming more than 3,500 researchers and commercial users was organized. Its objective was to share the cutting edge and experience in high-performance computing technologies and their utilization. At the fair with its 160 exhibitors, it has already been for the 6th time when we have presented our supercomputing infrastructure and the related research.

Our colleague Tomáš Martinovič, who presented his research work titled HPC Oriented Algorithm for Computation of Recurrence Quantitative Analysis at the conference poster section, was awarded the **Best Research Poster Prize**.

Moreover, the TOP 500 list of the most powerful supercomputers of the world was also announced and updated at the conference. Our four-year old Salomon supercomputer has remained in the list and was ranked 282nd.



Our colleagues at the ISC 2019 conference exhibition



Tomáš Martinovič with the Best Research Poster Award at the ISC 2019 conference

THE CZECH PRIME MINISTER VISITED US



WE WERE VISITED BY THE CZECH PRIME MINISTER

On Friday 17th May 2019, Andrej Babiš, the Prime Minister of the Czech Republic, visited us. During his hour long visit, we presented our centre, its operation, and also our engagement in international initiatives, projects, etc. The Prime Minister was primarily interested in our artificial intelligence research because, as he said, he considers it a research topic which is of enormous interest for the Czech Republic.



Photogallery from the visit: www.it4i.cz



