



NEWSLETTER Q4/2018

VSB TECHNICAL
UNIVERSITY
OF OSTRAVA

IT4INNOVATIONS
NATIONAL SUPERCOMPUTING
CENTER

Best Poster Award at the SC18 Conference won by an IT4I team

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We participated at the 30th annual Supercomputing Conference. The Best Poster Award was won by Ondřej Meca, Lubomír Říha, and Tomáš Brzobohatý for their contribution entitled Workflow for Parallel Processing of Sequential Mesh Databases.

Extension of the Anselm cluster

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At VŠB - Technical University of Ostrava an agreement for an upgrade of the HPC systems at IT4Innovations was signed in November 2018.

Our colleague Georg Zitzlsberger has become an ambassador of the NVIDIA Deep Learning Institute

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We plan to organize a whole-day training course on the topic of Deep Learning Fundamentals for Digital Image Processing.

The European Commission has nominated HyperLoom and the intelligent online navigation system for the Innovation Radar Prize

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Via online voting, the intelligent online navigation system has been shortlisted as one of four final candidates for the Innovation Radar Prize.

Evaluation of the 14th Open Access Grant Competition

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In September 2018, a total of 57.5 million core hours were distributed across 56 successful projects. We introduce selected projects awarded computational resources.

We have published a new publication entitled IT4Innovations Digital Innovation Hub

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In the online-available publication, you can learn about the particular examples of our cooperation with industry.

About the three conferences held at IT4I in November

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We have hosted the 3rd Day of National Research Infrastructure, the IT4Innovations Users Conference, and the Annual Conference of IT4Innovations Centre of Excellence.

Representatives of SMEs and business support organizations at IT4I

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Together with the Technical University of Košice, we have organized a seminar to raise awareness of the potential benefits of HPC for small and medium-sized enterprises.

IT4I and the public

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In 2018, we welcomed more than 1 700 visitors. Again, we participated in the Researcher's Night event and presented our infrastructure at the NATO Days.

IN BRIEF

**NEXT ROUND OF THE
OPEN ACCESS GRANT
COMPETITION TO
BE LAUNCHED IN
FEBRUARY 2019**

In February 2019, the 16th Open Access Grant Competition is to be launched for you to apply for the computational resources of IT4Innovations. For updates, see our website.

www.it4i.cz

TRAINING ACTIVITIES

For the updated portfolio of the training activities organized at our centre this year, please see the following link <http://training.it4i.cz/kurzy-it4innovations>. In March, for example, you can participate in the Parallel visualization of scientific data using Blender course.

<http://training.it4i.cz/kurzy-it4innovations>



Lubomír Říha
with the Best Poster
Award at the SC18
Conference

SC18
Dallas, TX | **hpc**
inspires.

BEST POSTER AWARD
AT THE SC18 CONFERENCE
WON BY AN IT4I TEAM



In November 2018, we participated at the **30th Supercomputing Conference (SC)**, which is the greatest global meeting of scientists and companies focused on the field of High Performance Computing (HPC). It was held at the Kay Bailey Hutchison Convention Center in Dallas (Texas, USA) and welcomed more than 13 thousand visitors.

The SC18 Best Poster Award was won by Ondřej Meca, Lubomír Říha, and Tomáš Brzobohatý

for their contribution entitled Workflow for Parallel Processing of Sequential Mesh Databases. Their poster was judged to be the best of almost 100 posters that were evaluated by the technical committee on the strength of the quality of the research, as well as its presentation.

We spoke to Ondřej Meca and Tomáš Brzobohatý

IT4I regularly participates at the SC conference, and in recent years the poster contributions of IT4I researchers have been shortlisted among the contributions nominated for the Best Poster Award. In past years, Asian contributions dealing with simulations of earthquakes were given this award. This year's winner was your contribution. Have you been stunned by this result?

"To be honest, we thought that again the award would be won by a contribution dealing with earthquakes or other related topic. We were all the more pleasantly surprised that we have finally managed to turn the several nominations of IT4I into winning the award itself."

Our contribution deals with seemingly trivial stuff, namely download of database files containing data of unstructured networks, which we develop massively parallel solvers for. In our research work, which is primarily driven by the requirements of our industrial partners, however, we often come across sequential formats of this data, which are originally not considered for parallel processing. Data in such formats are commonly used in the everyday engineering practice of many companies, and transition to a more suitable format seems to be unrealistic as it would often require significant

changes to the company structure. Until now, entry data must have been converted sequentially into a more suitable format, which was enormously time-consuming, and made efficient use of a supercomputing infrastructure much more difficult. Our solution overcomes this barrier and significantly accelerates both the conversion and direct download of sequential data and its preparation for distributed computing. The parallel scalability tests of our proposed approach show that it is possible to download and prepare sequential data consisting of hundreds of millions of unknowns within a few seconds. The conventional sequential processing, on the other hand, can take hours.

The solution we have developed allows direct connection to our industrial partners' data structure without the need for to intervene in their company structure, and transition to parallel formats. Using this approach, we aim to minimize all barriers for new potential users of HPC infrastructures and allow them to easily use the latest technologies available. The resulting solution is part of the massively parallel ESPRESO library, which has continually been developed by our team."



Our colleagues at the IT4Innovations booth at the SC18 conference

We also spoke to Lubomír Říha, who presented the contribution

The conference poster section took three days. It was also thanks to your efforts that the nomination turned into the award. Can you give us an idea about the way the technical committee proceeded in the process of selecting the best poster?

“Even though the poster section took three days, everything was decided within several minutes at Tuesday’s reception, which started at 5.15 pm local time and took two hours. This time, the technical committee gathered at the same time in about 20 minutes upon the commencement of the reception. The committee chairmen had introduced himself and announced that I had 7 minutes to explain the topic of our poster and its main contribution. This was the main difference in the practice from my experience in 2016, when we competed for the Best Poster Award in a very similar team. At that time, the committee members approached the contestants

alone, and as such we could talk for as long as they considered necessary. After less than ten minutes, each committee member had an opportunity to ask questions. They asked various questions such as where we planned to further publish this work, if our approach could be used in other scientific domains, what is our contribution as opposed to the state-of-the-art, etc. Fortunately, not a single question presented an unpleasant surprise.

The announcement itself took place during Thursday’s ceremony, when all conference awards were granted. The Best Poster Award was announced in the second half of the event, so I had to wait. The first fifth was quite rich with big names, such as NVIDIA, IBM, Oak Ridge National Laboratory, and the University of Erlangen-Nuremberg. Luckily, the right name was announced in the end.”

The six-day SC18 event was not only the venue of the conference, which included a poster section, lectures, workshops, discussion forums, et cetera, but also of an exhibition where hardware manufacturers, universities, and research organizations present themselves every year. It is a unique opportunity to gather the latest first-hand knowledge in the field of HPC, establish new contacts, and discover current global trends in HPC development.

Nearly 400 organizations from 26 countries presented their work at this year’s SC Exhibition. This has been the sixth consecutive year that IT4Innovations has participated at this event as an exhibitor. The visitors could thus learn more about our infrastructure as well as about the related research.

SC18 also featured the Birds of a Feather section, the aim of which is to provide space for discussions on the current issues facing HPC communities. At one such section, namely Strategies for Inclusive and Scalable HPC Outreach and Education, our centre was also represented.

Named after the pioneer of high performance and parallel computing, the most prestigious Gordon Bell Prize recognizing outstanding achievement in High Performance Computing was

awarded at the SC conference. The prize was awarded to two teams from USA. The Oak Ridge National Laboratory (ORNL) team succeeded with their article focused on the use of supercomputers in the fight with opioid epidemic. In cooperation with the US Department of Energy (DOE) and the US Department of Veterans Affairs, their research addresses the issue of prescribed opioids (e.g., morphine and codeine) abuse in the USA, and disorders developed therefrom not only in veterans. The ORNL team have developed a new algorithm, CoMet, which enables supercomputers to process a huge amount of genetic data as well as to identify the genes which increase our pain sensitivity and opioid addiction, and propose the most suitable medical treatment. CoMet is currently used in, for example, bioenergy and clinical genomics projects. The second awarded contribution was Exascale Deep Learning for Climate Analysis, presented by the Lawrence Berkeley National Laboratory team. Using supercomputers, they teach deep neural networks to identify extreme climate phenomena, such as tropical cyclones and atmospheric rivers, from simulations of high-resolution climate models.

Moreover, an updated TOP500 list of the world's most powerful supercomputers was announced at the conference. Being already its 52nd edition, it contains the list of the world's 500 most powerful supercomputers with the aggregate theoretical peak performance of 2 200 Pflop/s. A total of 153 brand new systems, 15 of which are operated in Europe, have been added to the list.

The list has been dominated by China with almost half of the supercomputers (229) with an aggregate theoretical peak performance of 810 Pflop/s. The United States of America operate a total of 108 systems (755 Pflop/s), Japan 31 systems (170 Pflop/s), the United Kingdom 20

(52 Pflop/s), France 18 (66 Pflop/s), and Germany 17 (86 Pflop/s) systems included in the list

In the TOP500 list, information about the particular sector where each supercomputer falls is also included. These segments are, in particular, academia, government, research, industry, and others (manufacturers of supercomputers and other non-specified ones). The current TOP500 list shows that more than 50 % and approximately 30 % of the theoretical peak performance of the supercomputers worldwide is used in research and industry, respectively. A total of 10 % is used in academia and another 10 % in government and other

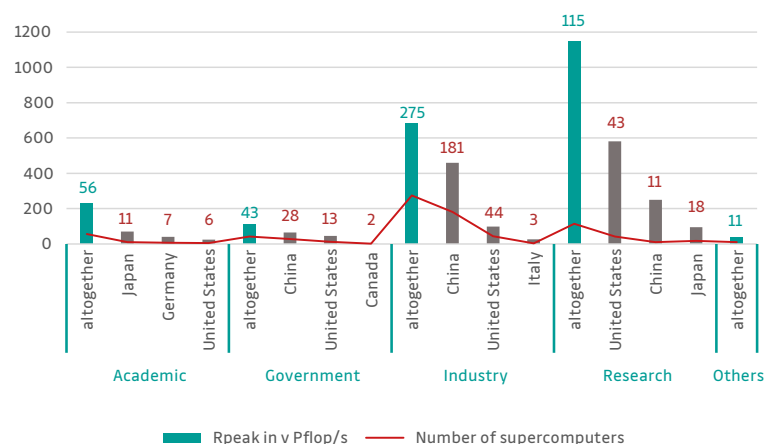
(e.g. manufacturers of supercomputers). The highest number of supercomputers (275) is used in industrial practice.

The computational resources of the computing systems operated at IT4Innovations are primarily provided to Czech research institutions and universities within Open Access Grant Competitions. Let's have a closer look at the situation in academia reflected in the TOP500 list.

This segment is dominated by Japan with its number of systems as well as aggregate theoretical peak performance. However, the first place is occupied by SuperMUC-NG, the new German

supercomputer installed at the Leibnitz Supercomputing Centre (LRZ) and to be made available to users in January 2019. With nearly 6.5 thousand compute nodes and a total of more than 300 thousand cores, its theoretical peak performance is 27 Pflops/s. With its theoretical peak performance of 2 Pflops/s (1 008 compute nodes and 76 thousand cores), the Czech Salomon supercomputer ranked 13th in the academic segment.

TOP500 list and its segments



The first thirteen European supercomputers used in academia and included in the TOP500 list

Supercomputer	Country	Ranking in the TOP500 list in November 2018	Linpack benchmark performance in Pflop/s
SuperMUC-NG	Germany	8	19.48
Marconi Intel Xeon Phi	Italy	19	10.38
MareNostrum	Spain	25	6.47
SuperMUC	Germany	64	2.9
SuperMUC Phase 2	Germany	65	2.81
occigen2	France	77	2.5
Lomonosov 2	Russia	79	2.48
Cumulus	Great Britain	87	2.27
Mogon II	Germany	99	1.97
Beskow	Sweden	111	1.8
Marconi Intel Xeon	Italy	122	1.72
Prometheus	Poland	131	1.67
Salomon	Czech Republic	213	1.46





EXTENSION OF THE IT4I CLUSTER



The signing of the agreement for the upgrade of HPC systems for IT4Innovations on 9th November 2018

At VŠB - Technical University of Ostrava, an agreement for the upgrade of HPC systems for IT4Innovations National Supercomputing Center was signed on 9th November 2018. It includes extension of the Anselm cluster with a theoretical peak performance exceeding 800 Tflops/s (thus becoming 8 times more powerful than the currently operated system launched in 2013). This extension will be provided by Atos IT Solutions and Services, s.r.o.

In the challenging competitive dialogue, eventually won by the Atos company, emphasis was placed not only on the price but also use of currently available state-of-the-art technologies. Czech scientists will thus have access to the latest generation of Intel processors as well as to the most powerful NVIDIA GPU accelerators.

“The demand of Czech scientists for computational resources exceeds our currently available capacity by about 100 %. This upgrade will increase our capacity and help us address this problem. At the same time, Czech scientists will get access to state-of-the-art technology, enabling them to keep up with the rest of the world”, said Vít Vondrák, the Managing Director of IT4Innovations.

Based in Ostrava, IT4Innovations caters for the computational resource needs of scientists from both Czech universities and prestigious research centres. More than 50 % of the supercomputers' capacity is used for novel materials and drug design, with the remaining capacity being used for biosciences, engineering problems, astrophysics, and other scientific fields.

IT4Innovations computing capacity extension was supported by the European Regional Development Fund in the IT4Innovations National Supercomputing Center – Path to Exascale project No. CZ.02.1.01/0.0/0.0/16013/0001791 within the Operational Programme Research, Development and Education of the Ministry of Education, Youth and Sports.

The upgraded part of the system will be equipped with a total of 198 compute nodes: 189 standard compute nodes (2x 12-core Intel processors and 192 GB RAM in each node), 8 compute nodes with GPU accelerators (2x 18-core Intel processor, 4 NVIDIA V100 GPU accelerators with 16 GB GPU and 192 GB RAM in each node), and a fat node (4x 12-core Intel processors and 6 TB RAM). The supercomputer will be built on the BullSequana X HPC

architecture, and standard node cooling will be based on direct liquid cooling. The computer network will be based on the latest Infiniband HDR technology. Data storage for SCRATCH computations will have a capacity of 200 TB and a 28 GB/s throughput accelerated by Burst Buffer technology. Data storage for NVMe over Fabric computations will have total capacity of 22.4 TB dynamically allocated to compute nodes. Bull Super Computer Suite, the PBS Pro resource planner and manager, will support the software solution for operation and administration of the cluster.

NVIDIA DEEP LEARNING INSTITUTE CERTIFICATE OF COMPETENCY

This certificate is awarded to
GEORG ZITZLSBERGER
for demonstrating competence in the completion of
**FUNDAMENTALS OF DEEP
LEARNING FOR COMPUTER VISION**



Will Ramey

Director of The NVIDIA Deep Learning Institute, NVIDIA

2018
Year issued



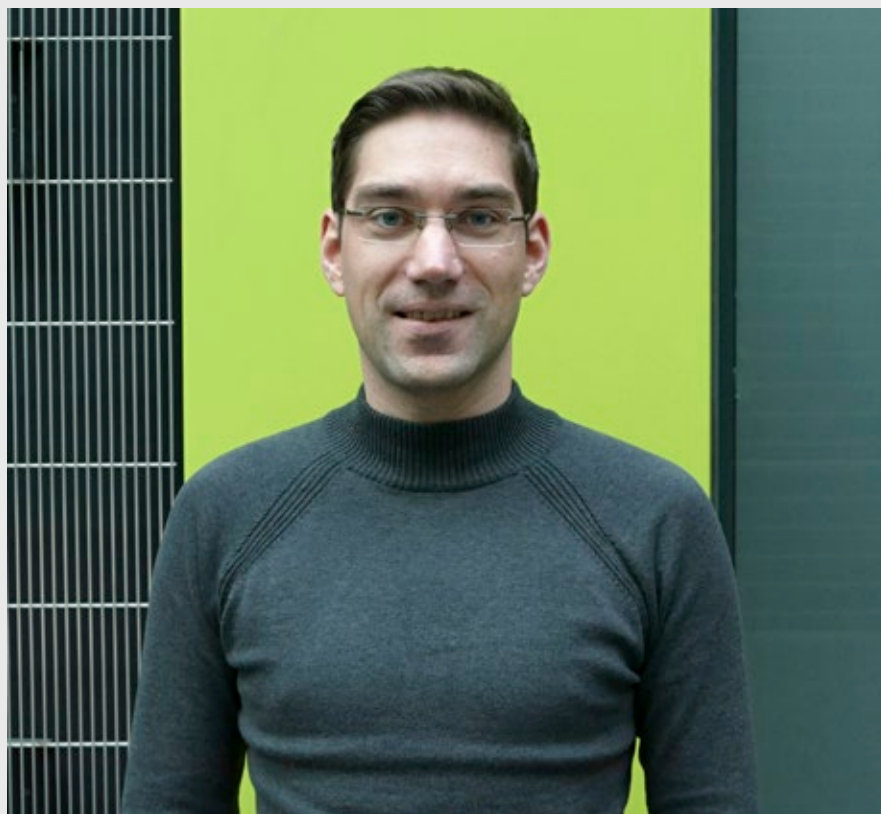
DEEP
LEARNING
INSTITUTE

GEORG ZITZLSBERGER HAS BECOME
AN AMBASSADOR OF THE NVIDIA
DEEP LEARNING INSTITUTE

In the context of the planned capacity extension of the Anselm cluster with the latest NVIDIA GPU accelerators, we are pleased to announce that thanks to our colleague Georg Zitzlsberger IT4Innovations has received NVIDIA Deep Learning Institute Ambassador status. Mr. Zitzlsberger obtained the NVIDIA Deep Learning Institute (DLI) instructor certificate at the end of 2018.

The NVIDIA Deep Learning Institute offers practical courses to developers and researchers who would like to solve complex problems using deep learning methods. The institute provides training courses led by certified instructors on the latest methods for designing, teaching, and deploying machine learning based on neural networks in various areas of application. Participants of the courses explore the widely-used open-source tools and latest platforms for deep learning accelerated by NVIDIA GPU processors.

Our colleague Georg Zitzlsberger



We spoke to Georg Zitzlsberger

Congratulations on your certification. What course can we look forward to this year?

"Thank you. It also is a pleasure for me to announce that with the certification, IT4Innovations became a part of the NVIDIA Deep Learning Institute (DLI) programme and also received NVIDIA University Ambassador status. Within the Visegrad region, IT4Innovations is one of the first institutes to receive this status. IT4Innovations as an NVIDIA Deep Learning Institute is a great opportunity for our users to receive high quality training courses from NVIDIA, and benefit from our extended services around the latest NVIDIA architectures for HPC and deep learning.

The first certification acquired from NVIDIA covers the full day training course "Fundamentals of Deep Learning for Computer Vision". It educates software developers and researchers about how to apply deep learning for computer

vision problems. Tutorials explain how to implement common deep learning workflows, such as image classification and object detection. The training course also teaches how to experiment with data, training parameters, and network structure, and other strategies to increase network performance and capabilities as well as how to deploy neural networks to start solving real-world problems. We plan to offer this course in the first half of 2019, along with NVIDIA services offered by our new cluster.

This first certification is just the starting point of a longer collaboration with NVIDIA. We expect more certifications to come in 2019, which will extend our offered training courses with CUDA/OpenACC programming, and deep learning for multiple GPUs."

For more information, please see the courses website.



EUROPEAN COMMISSION HAS NOMINATED
HYPERLOOM AND THE INTELLIGENT ONLINE NAVIGATION
SYSTEM FOR THE INNOVATION RADAR PRIZE

The Innovation Radar is an initiative of the European Commission whose objective is to identify European innovators and innovation acts that have been supported by European projects in the information and communication technology field. This year, the initiative selected 48 best innovation acts, which were divided into 5 categories. Two achievements of our colleagues from the Advanced Data Analysis and Simulations Laboratory were nominated in two categories.

In the Excellent Research category, the HyperLoom software enabling easy parallel data processing was nominated. HyperLoom enables its users to efficiently define dependencies of up to millions of interconnected computational tasks and create a pipeline which is then efficiently executed using a supercomputer. The software has been used, for example, to execute pharmaceutical and civil engineering problems.

In the Innovation category, the intelligent online navigation system for citizens in its early stage was nominated and shortlisted with three other finalists thanks to online voting. We have cooperated on this system with the company Sygic, with the objective of mitigating traffic congestion. Using supercomputers, the navigation system can provide drivers with the most up-to-date data available in the shortest time possible for a total drive time reduction.

A total of 20 finalists gathered in Vienna at ICT 2018 at the beginning of December to present their innovations to the technical committee. The winner of the Innovation Radar Prize was Gr3n from Switzerland for their PET waste upcycling technology.



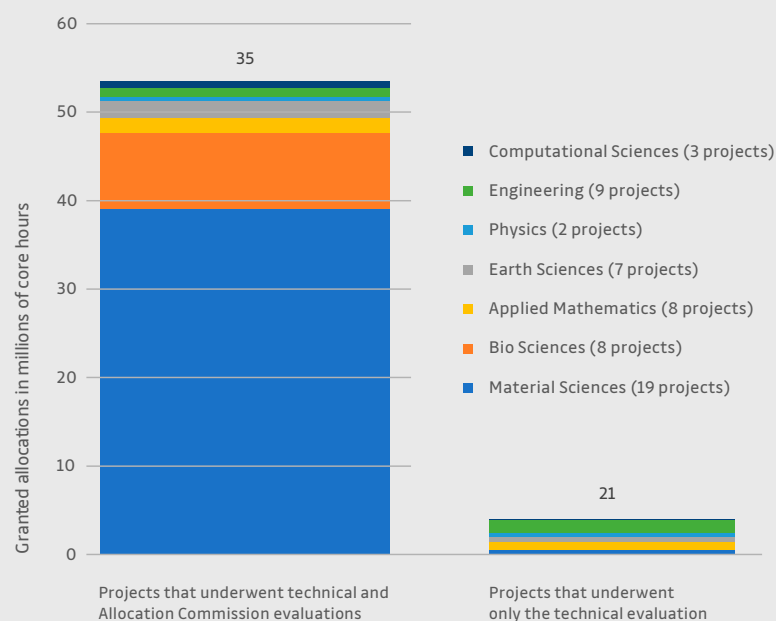


EVALUATION OF THE 14th OPEN ACCESS GRANT COMPETITION



Within the 14th Open Access Grant Competition applicants applied for more than 93 million core hours. The demand for our computational resources exceeded the reserved capacity, which amounts to 48 million core hours, by 94 %. The allocation committee was thus forced to decrease the amount of computational resources granted to most projects. Within the 14th Open Access Grant Competition, a total of 57 541 000 core hours were eventually allocated across 56 successful projects.

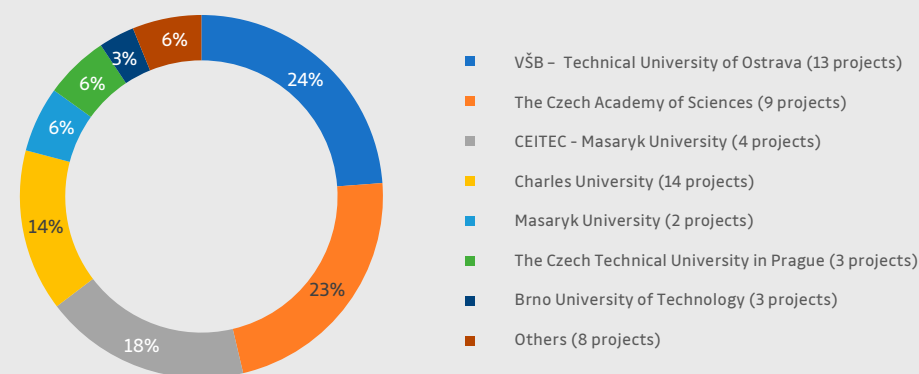
All in all, 93 % of the allocated computational resources were granted to 35 projects, which passed the technical evaluation as well as the evaluation of the allocation committee. The most represented scientific domain was material sciences (17 projects) followed by biosciences (8 projects). Altogether 15 projects were granted an allocation of more than 1 million core hours each. The investigators of these projects are the researchers of IT4I, Czech Academy of Sciences, CEITEC, Charles University, Masaryk University, and Czech Technical University in Prague.

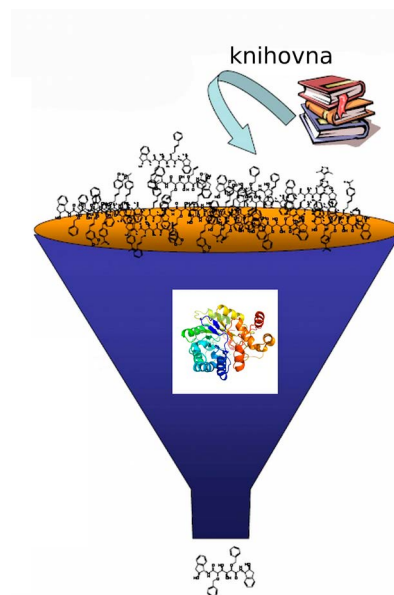


The projects of applicants who applied for 400 thousand core hours or less had to pass the technical evaluation only, and the required resources were allocated to them in full. These 21 projects were granted a total of 7 % of the total number of allocated core hours. The majority of the projects fall in the categories of engineering research (7 projects) and applied mathematics (5 projects).

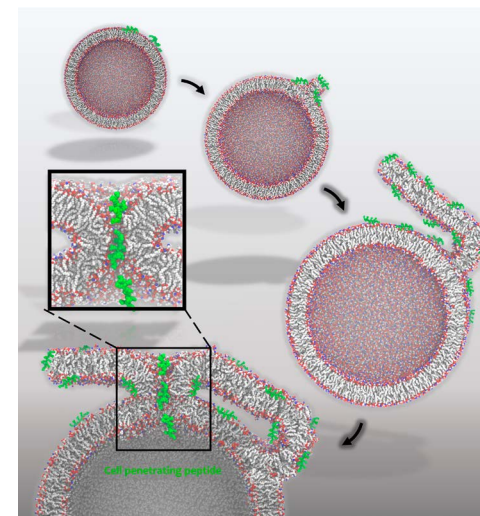
Regarding the distribution of resources amongst organisations, a quarter of the total allocated computational resources was awarded to the projects of VŠB-TUO (primarily IT4Innovations) applicants. Another quarter of these resources was awarded to projects from Czech Academy

of Sciences institutes. The majority of projects successful in the 14th Open Access Grant Competition are from Charles University. A total of 14 projects of this university were awarded more than 8 million core hours. Additionally to the projects of the universities and research institutions presented in the graph above, 3 projects of the Czech Aerospace Research Centre as well as projects of the University of Chemistry and Technology Prague, the University of Ostrava, Tomáš Baťa University in Zlín, Palacký University Olomouc, and the University of Pardubice, with each of them having one project, were awarded computational resources.





Virtual screening



Cell-penetrating peptide

Prof. Ing. Pavel Hobza, DrSc., FRSC
The Czech Academy of Sciences

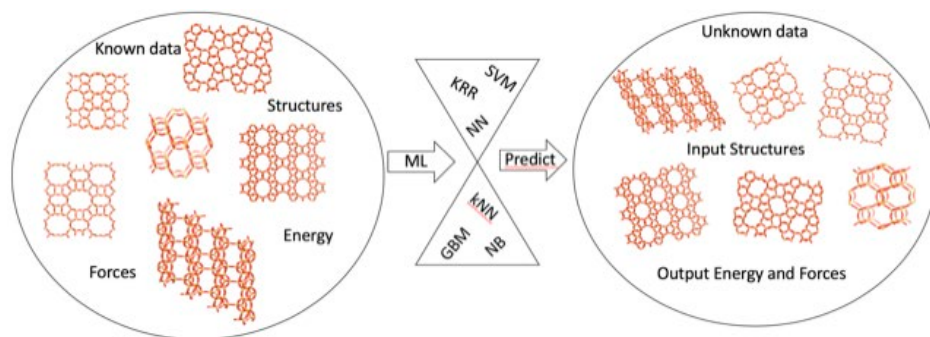
IN SILICO DRUG DESIGN

The Principal Investigator of the project focused on development of in silico drug design methods is Pavel Hobza from the Czech Academy of Sciences. This is his ninth project involving the use of a supercomputer, which was awarded IT4Innovations computational resources. The objective of his research group's work is to develop a reliable computing strategy for identification of new ligands, which bind to therapeutically relevant proteins such as HIV protease, cyclin-dependent kinases, and aldo-keto reductases. The team is currently focused on developing reliable protocols for the virtual screening of compound libraries, which may contain millions of chemical substances. For the project of virtual screening for drug discovery, the team of professor Hobza was awarded more than 6 million core hours this time.

Prof. Mgr. Pavel Jungwirth, CSc., DSc.
The Czech Academy of Sciences

EFFECTS OF BIOMECHANICAL PROPERTIES OF LIPID MEMBRANES

Prof. Pavel Jungwirth from the Institute of Organic Chemistry and Biochemistry of the CAS focuses on the research of macroscopic properties of lipid membranes. Aided by a supercomputer and molecular dynamics methods, he will perform a simulation of lipid bilayer behaviour. In plasma membranes, not only their chemical composition (e.g., types of the membrane-forming lipids) but also their shape will be investigated. The team of Prof. Jungwirth aims to detect the effects of the bilayer shape on membrane interactions. New findings about membrane shapes will open new opportunities for understanding the regulation of enzymes and other proteins in cells.

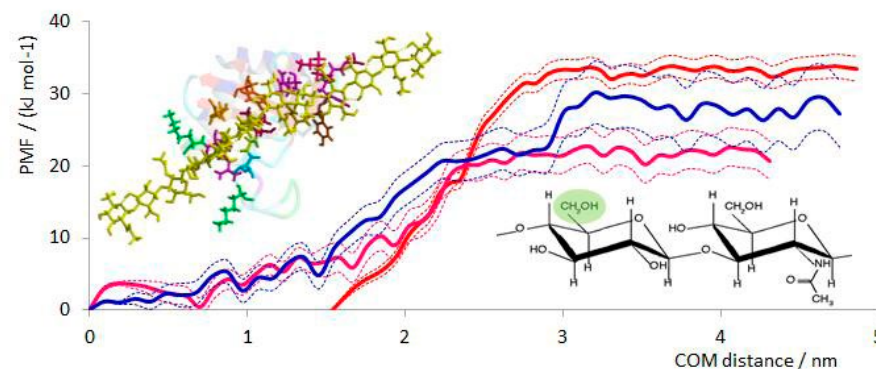


A machine learning approach for the description of zeolites

Mgr. Miroslav Rubeš, Ph.D.
Czech Academy of Sciences

A MACHINE LEARNING APPROACH FOR THE DESCRIPTION OF ZEOLITES

The scientific domain with projects with the highest allocation of computational resources not only in our centre is material science. The project of Miroslav Rubeš from the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, which was awarded almost 2 million core hours, falls in this domain as well. It is focused on zeolites, which are used as detergents, catalysts, and adsorbents. In 2017, the value of the global zeolite market was about 30 billion US dollars. The objective of Miroslav Rubeš project is to use machine learning algorithms to create a model which enables deeper understanding of the phenomena occurring in zeolitic materials..

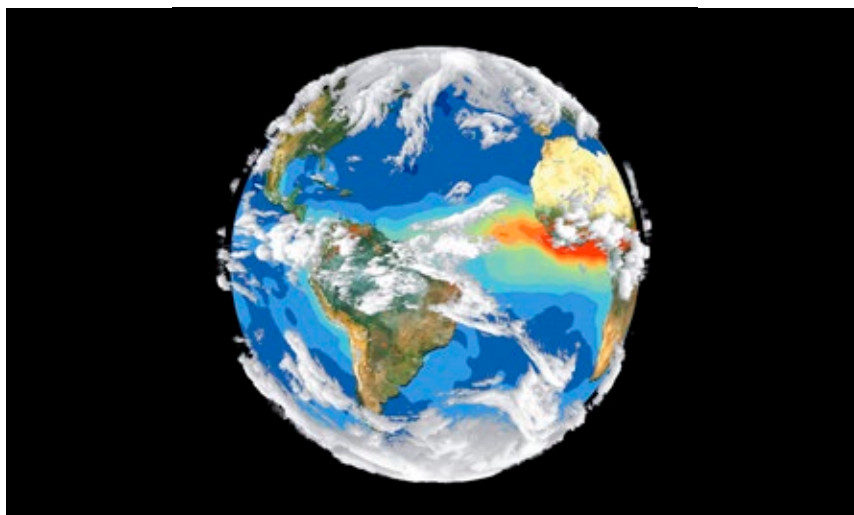


Adaptive biasing force dependency on the distance between the ligand and receptor ground state (Link of the TSG-6 protein domain) calculated by means of the umbrella sampling method (the dotted lines indicate standard deviation). The ligand represented here is hyaluronic acid oligosaccharide (red, 2 different binding sites) or its neutral analogue containing glucose instead of glucuronic acid (blue, 1 binding site).

RNDr. Marek Ingr, Ph.D.
Tomáš Baťa University in Zlín

HYALURONAN STRUCTURE, INTER-MOLECULAR INTERACTIONS AND INTERACTIONS WITH PROTEIN RECEPTORS

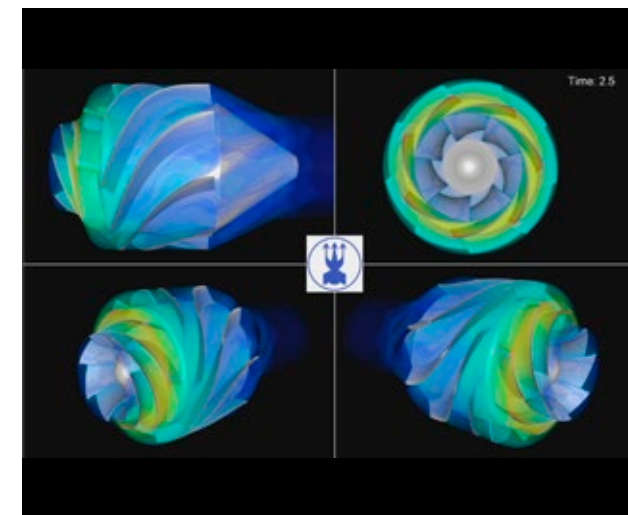
Hyaluronic acid is a natural polysaccharide present, for example, in connective tissues and synovial fluid. It performs a large number of biological functions and is used not only in cosmetics but also in the healthcare sector in osteoarthritis treatment and wound and burn care. Hyaluronic acid reacts with protein receptors and mediates cellular signalling amongst other functions. Therefore, it is assumed that it also plays its part in the development of various diseases, including cancer. Research of hyaluronic acid and the mechanism of its molecular interactions with protein receptors is also carried out by Marek Ingr from Tomáš Baťa University in Zlín, who was awarded computational resources in our 12th as well as 14th Open Access Grant Competitions. He uses a supercomputer to perform molecular dynamics simulations with the aim to detect, for example, the key hyaluronan-protein interactions. Building on these findings, new drugs and cosmetic products may possibly be designed.



Mgr. Michal Belda, Ph.D.
Charles University

CONVECTION PERMITTING CLIMATE SIMULATIONS

In climate change assessment, global and regional climate models are an important tool. However, they still have relatively low resolution, and their potential to be used for local application is therefore limited. The low resolution of the majority of models does not allow implicit assessment of phenomena such as upward movements (convection) and the resulting intensive precipitations. In models, these phenomena need to be parametrically represented. Since 2016, researchers from almost 30 European institutions have been cooperating on a pilot study approved by the advisory team of the World Climate Research Programme (WCRP). For developing climate scenarios, this study uses regional non-hydrostatic high-definition (3 km and less) implicit convection permitting modelling. In the future, we will thus have much more detailed scenarios of climate change effects on the regional and local level. In our 14th Open Access Grant Competition, Michal Belda from Charles University, who is involved in this WCRP pilot study, was awarded 1 million core hours for the simulation of long-term climate in the past in order to serve as a base for assessment of future climate scenarios. Belda will focus on the Alpine region and the Czech Republic.



CFD simulation
of water pump

Mgr. Tomáš Krátký
Palacký University Olomouc

AN OPEN-SOURCE BASED FRAMEWORK FOR CFD-BASED OPTIMIZATION OF ROTARY MACHINES

Tomáš Krátký from Palacký University Olomouc was awarded half a million core hours for the development of a fully automated model for CFD-based rotary machine simulations. Solely based on open source software (OpenFOAM, Python), this brand new model will allow designers to optimize the shapes of rotary machines to achieve their best possible hydraulic performance. They will thus achieve better designs of rotary machines in a shorter time.

The new computational approach will be used in pump design, which is expected to outmatch the currently used ones by its performance parameters. Research and development in the field of numerical simulation for shape optimization plays a key role for pump and turbine manufacturers. Drawing the benefits of a faster and cheaper computational approach for hydraulic designs, companies may thus optimize and tailor their products for their customers.

WE HAVE PUBLISHED A NEW
PUBLICATION ENTITLED IT4INNOVATIONS
DIGITAL INNOVATION HUB



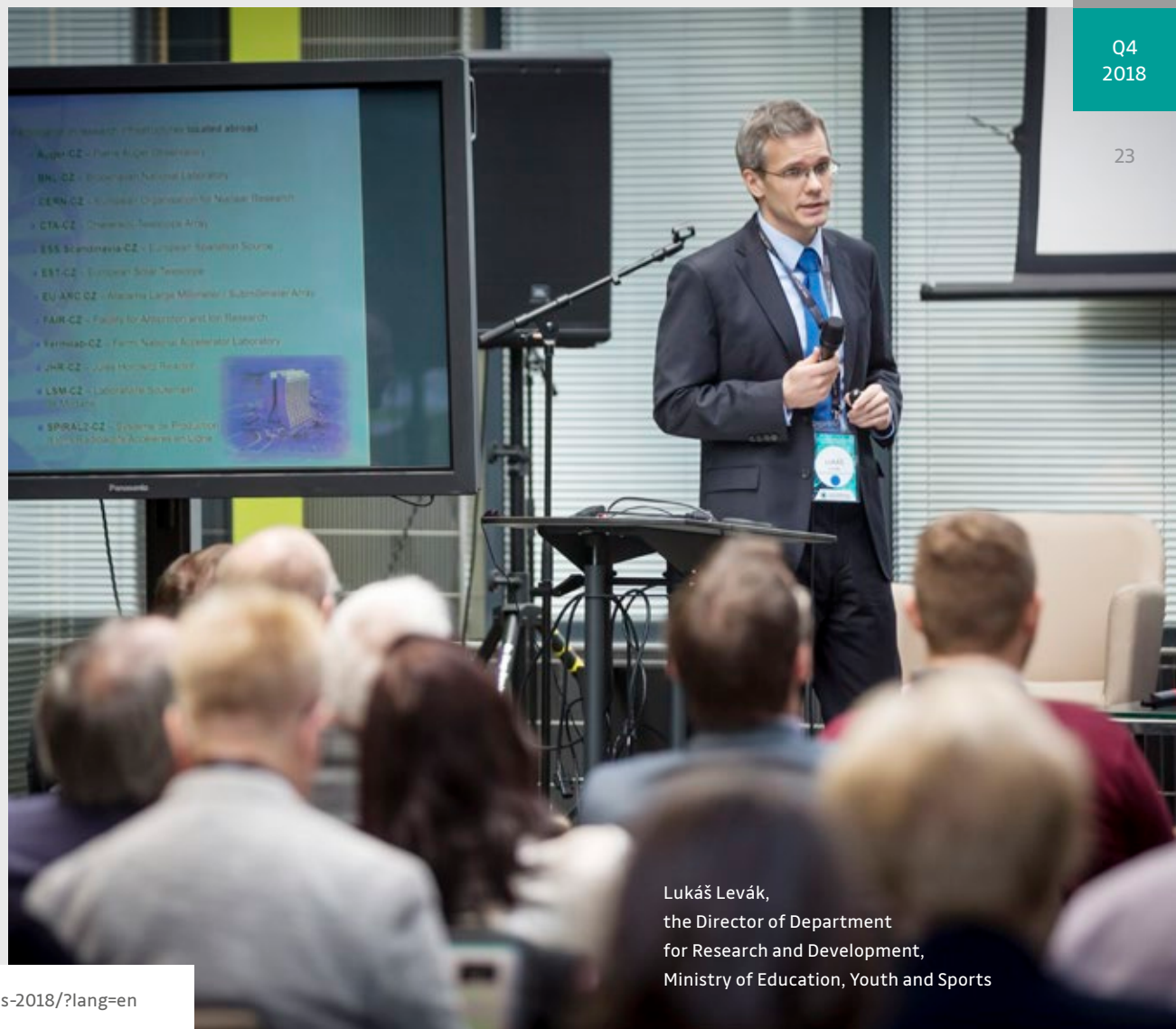
ABOUT THE THREE
CONFERENCES HELD
AT IT4I IN NOVEMBER

DAY OF NATIONAL RESEARCH INFRASTRUCTURES 2018

In 2018, the 3rd Day of National Research Infrastructures was held at our centre. Welcomed by Branislav Jansík, the Head of the Supercomputing Services, nearly 100 people gathered to participate in technical discussions on crucial current issues in policy making and funding of large research infrastructures in the Czech Republic. Lukáš Levák, the director of the Department for Research and Development of the Ministry of Education, Youth and Sports made an appearance at the conference, where he presented the Research Infrastructures (RI) financial framework for the years 2020–2022.

The financial framework reflected the results of the international evaluation from 2017, the subject of which was 58 RI as well as 17 newly submitted proposals for RI. 21 existing infrastructures were evaluated as 'excellent' including IT4Innovations and 3 new proposals for RI. 24 RI and 4 proposals were evaluated as 'very good'. As of the year 2020, 7 infrastructures will merge into 3 projects. One of them is represented by a single e-infrastructure, which will be established by merging IT4Innovations with CESNET and CERIT-SC (e-INFRA CZ).

Funding for 48 research infrastructures from public funds of the Czech Republic for the period up to the year 2022 was approved on 12th December 2018. The targeted support provided by MEYS annually amounts to CZK 1.89 billion, and the total investment aid, which can be drawn from the calls of the Research, Development and Education Operational Programme, will amount to CZK 3 billion. Following the changes in RI, MEYS aims to update the Roadmap of Large Infrastructures for Research, Experimental Development and Innovation of the Czech Republic.



Lukáš Levák,
the Director of Department
for Research and Development,
Ministry of Education, Youth and Sports

<https://www.it4i.cz/portfolio/day-of-national-research-infrastructures-2018/?lang=en>

<https://www.vyzkumne-infrastruktury.cz/en/events/day-of-national-research-infrastructures-2018/>

IT4INNOVATIONS USERS CONFERENCE

At the 2nd IT4Innovations Users Conference we hosted almost 100 attendees who had an opportunity to listen to contributions from various scientific domains and exchange their user experience. The research projects of our colleagues as well as of the external users of the IT4Innovations infrastructure, for example, from the Czech Academy of Sciences (CAS), CEITEC, Charles University, the University of Chemistry and Technology Prague, the Czech Technical University in Prague, and Tomáš Baťa University in Zlín, were presented. The conference programme included 20 talks as well as a poster section for presentation of research projects.

<https://events.it4i.cz/event/11/>

www.it4i.cz/portfolio/2nd-users-conference-of-it4innovations-2018/?lang=en



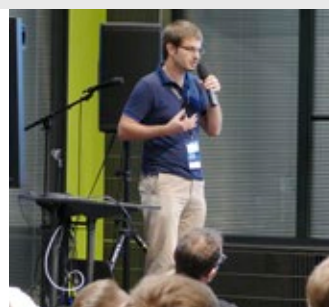
RICHARD WÜNSCH

Some notable examples which were heard at the conference included two contributions of users from the Astronomical Institute of the CAS. Richard Wünsch presented his research on the Origin of globular clusters: Star formation in the most extreme conditions. Using our supercomputer, his team simulated the formation of second-generation stars. They developed a model to demonstrate the formation of second-generation stars in globular clusters from the material of the star winds - the particle stream that escapes from the atmosphere of the first generation stars.



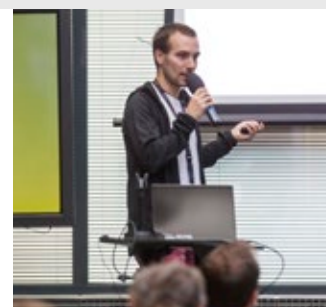
TAYLOR RHYS

Taylor Rhys talked about the research of optically dark clouds of neutral hydrogen in the Virgo galaxy cluster. He used the Salomon supercomputer for a series of simulations modelling the turbulent cloud development. The result of his research project is a finding that a stable state cannot arise in the proposed system. Depending on the initial conditions, the cloud starts to collapse or form stars in a relatively fast manner.



JIŘÍ KLIMEŠ

Jiří Klimeš from the Faculty of Mathematics and Physics at Charles University in Prague presented the methods he applies for calculating the properties of molecular solids. They play an important role in nature and industry alike. His research group uses the Salomon supercomputer, for instance, to calculate the binding energies of selected molecular crystals.



MICHAL H. KOLÁŘ

Michal H. Kolář from the University of Chemistry and Technology Prague contributed to the conference programme with his talk in the field of biology, namely on the topic of ribosomes and the VemP protein, the structural and dynamical properties of which he studies, amongst other things, using the Salomon supercomputer.



STELLA SKIADOPOULOU

Our colleague Stella Skiadopoulou presented her contribution in the field of material science, focused on magnetoelectric multiferroics, a promising candidate for use in new hybrid technologies. She presented a study of dynamic magnetoelectric coupling in selected polar antiferromagnets by combining several approaches, including HPC.

ANNUAL CONFERENCE OF IT4INNOVATIONS CENTRE OF EXCELLENCE

On Thursday 8th November 2018, the regular meeting with the partners of the IT4Innovations Centre of Excellence (2011–2015), namely the University of Ostrava, Brno University of Technology, the Silesian University in Opava, and the Institute of Geonics of the Czech Academy of Sciences, was held at our centre. Our cooperation with these partners continues in the sustainability period in the form of the National Programme of Sustainability II (2016–2020). At the 7th Annual Conference of IT4Innovations Centre of Excellence, the partners' representatives presented the main research orientation and research results of their research programmes in the last year.

<http://ce.it4i.cz>

www.it4i.cz/portfolio/7th-annual-conference-of-it4innovations/?lang=en



REPRESENTATIVES OF SMEs
AND BUSINESS SUPPORT
ORGANIZATIONS AT IT4I

On Monday 24th September 2018, we organized the HPC for small and medium enterprises workshop in cooperation with the Technical University of Košice. Its objective was to raise awareness of the potential benefits of HPC among small and medium-sized enterprises (SMEs). A total of 17 SMEs and business support organizations representatives participated at the workshop.

The workshop was supported from the High-performance Computing for Efficient Innovation in the Danube Region (InnoHPC, DTP1-I-260-I.1.) project of the Interreg Danube transnational programme co-funded from European Union funds (ERDF, IPA).

The participants acquired knowledge about the latest trends in HPC as well as about the competence of both Czech and Slovak HPC centres to support innovation development in small and medium-sized enterprises using supercomputers. Our colleague Tomáš Karásek, and Filip Holka from the Centre of Operations of the Slovak Academy of Sciences presented selected success stories of the cooperation of such enterprises with HPC centres. In addition, Martin Dujčák from the Technical University of Košice spoke about possible models of cooperation, and possibilities for the funding of innovations.



**In the year 2018, our centre
received more than 1700 visitors.**

They visited us for various reasons such as excursions, workshops, public events, etc. In the final months of the year, we opened the doors of our institute to the public for the Researcher's Night event, and presented our unique infrastructure at the NATO Days.

IT4I AND THE PUBLIC



RESEARCHER'S NIGHT

On Friday 5th October 2018 Researchers' Night took place in more than 30 places all over the Czech Republic. It is a scientific and technology promoting event, which offers the public a unique opportunity to have a taste of science in an entertaining way. This year's National coordinator of the event with more than 60 thousand attendees was a group of three institutions from Ostrava (VŠB-TUO, the University of Ostrava, and the Lower Vítkovice Area – Science and Technology Center).

This is the third time we have participated in the event, receiving a total of 732 visitors who were presented with a smart fun-packed programme. Over the course of the 5 hours that the doors of our institute were open to the general public, visitors had an opportunity to listen to the talks of several scientists. For example, Pavel Tomančák from the Max Planck Institute in Dresden (Germany) talked about developing a software application for microscope image processing using supercomputers. Jiří Jaroš from Brno University of Technology shared new findings in the development of computer-aided ultrasound diagnostics for brain surgery and stimulation. Karel Janko from the Czech Academy of Sciences/the University of Ostrava told visitors about the research of clonal reproduction in nature, and problems his team tries to solve with the use of a supercomputer. Finally, the last talk, about the key challenges of lithium metal batteries faced by scientists, was presented by our colleague Dominik Legut.

The visitors had an opportunity to see our supercomputing infrastructure and learn about the demands related to the operation of supercomputers. For children, and not only for them, we prepared a game consisting of five tasks, which the visitors with children regarded as the most attractive part of the programme. Moreover, they could play computer games such as Mars Mania and Shooting Stars as well as learn about PRACE, the pan-European research infrastructure, the objective of which is to increase the competitiveness of European science, research, and industry.

<https://www.it4i.cz/portfolio/researchers-night-2018/?lang=en>



NATO DAYS

It is the second time we have presented the IT4Innovations infrastructure and our research at the NATO Days in Ostrava, the largest security show in Europe. With some 220 thousand visitors coming to the show, the 18th NATO Days were also dedicated to commemoration of the 100th anniversary of Czechoslovakia. The weekend programme included not only dynamic displays of air and ground forces equipment but also booth presentations of the NATO Days partners.

The weather was on our side, and we had an opportunity to attract a countless number of visitors. The aim of our participation at the show was to increase awareness of IT4Innovations. The visitors had a unique opportunity to take a virtual tour around the data room, and see the Permonik cluster along with its larger successor.



