



Dear friends of supercomputing,

this is the last newsletter of the year 2017. We would like to thank you for your continuing support and that you supercompute with us. As in previous years, we have argued the case for the scientific community in the Czech Republic to keep having access to high-performance computing resources and services related to them. In 2017, we have succeeded in defending the crucial IT4Innovations National Supercomputing Center – Path to Exascale project, which will enable us to further develop and upgrade our infrastructure. The cluster Anselm will be upgraded at the end of 2018 and the cluster Salomon in 2020. I hope that the new systems will enjoy at least the same interest as the existing ones.

I wish you a successful year in 2018.

Vít Vondrák
IT4Innovations Managing Director



Results of the 11th Open Access Grant Competition

Altogether 54,999,384 core hours have been allocated across 51 successful projects. Most of the computational resources, 74 % of all the computational resources allocated within this call, have been allocated to projects in the field of material sciences. Allocated resources are available to users from September 2017 to June 2018.

[Read more](#)



The 6th Annual Conference of IT4Innovations and the 1st IT4Innovations Users Conference, and an Interview with Paolo Nicolini, the Chairman of the Executive Board of the IT4I Users Council

At the end of October, we organized two conferences. At these occasions, the IT4I Users Council was also established. The new Chairman of the Executive Board of the Users Council Dr. Paolo Nicolini provided us with an interview.

[Read more](#)



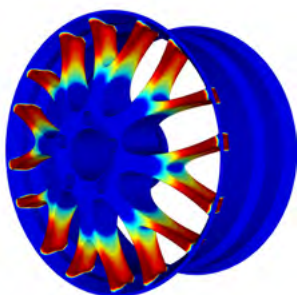
Participation at the Supercomputing Conference SC17 in Denver, USA

In November, we participated at the most important conference in the field of supercomputing technologies.

[Read more](#)

The students of Computational Sciences do not let the grass grow under their feet, and discover the world thanks to the prestigious summer schools

Our students took part in three prestigious international summer schools this year.

[Read more](#)

ESPRESO FEM – Heat Transfer Module

The development team of the massively parallel library ESPRESO has recently completed a module for solving heat transfer problems.

[Read more](#)

Partnership with Bayncore

In November 2017 IT4Innovations initiated a partnership with Bayncore from the United Kingdom.

[Read more](#)

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The next Open Access Grant Competition will be launched at the beginning of February 2018

At the beginning of February 2018, the 13th Open access grant competition will be launched, where you will be able to apply for the computational resources of our supercomputers. Watch the news on our website.

[More info](#)

INVITATIONS

InfiniBand, Omni-Path, and High-Speed Ethernet for Dummies

This workshop is the basic one from two half-day long workshops on interconnection technologies for high-performance computing systems. This workshop will provide an overview of InfiniBand (IB), Omni-Path, and High-speed Ethernet (HSE) technologies, their specific features, comparison of these technologies and their suitability for building clusters, cloud platforms and big data environments. The tutor Prof. Dhableswar K. Panda from Ohio State University is one of the most prominent experts in this field and his team develops interconnection subsystems implemented on the most powerful supercomputers.

When: **23 January, 2018** | Venue: VŠB – Technical University of Ostrava, IT4Innovations National Supercomputing Center
Level: Beginner-intermediate
Tutors: Dhableswar K. Panda, Hari Subramoni (The Ohio State University)

[More info](#)

InfiniBand, Omni-Path, and High-Speed Ethernet: Advanced Features, Challenges in Designing, HEC Systems and Usage

This on-going half-day workshop will be focused on advanced hardware and software features of IB, Omni-Path, HSE, and RDMA over Converged Enhanced Ethernet. Also included will be Open Fabrics RDMA and Libfabrics programming, and network management infrastructure and tools to effectively use these systems. Case studies, their solutions and sample performance numbers will be presented too.

When: **23 January, 2018** | Venue: VŠB – Technical University of Ostrava, IT4Innovations National Supercomputing Center
Level: Intermediate-advanced
Tutors: Dhableswar K. Panda, Hari Subramoni (The Ohio State University)

[More info](#)

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High Performance Distributed Deep Learning

In this third workshop tutorial Prof. Dhabaleswar K. Panda and his colleague Hari Subramoni will provide an overview of interesting trends in Deep Learning (DL) and how cutting-edge hardware architectures are playing a key role in moving the field forward. Included will be an overview of DL frameworks from an architectural as well as a performance standpoint and new challenges for MPI runtimes to efficiently support Deep Neural Networks (DNN) training. Tutors will highlight how they designed efficient communication primitives in MVAPICH2 to support scalable DNN training.

When: **24 January, 2018** | Venue: VŠB – Technical University of Ostrava, IT4Innovations National Supercomputing Center

Level: all levels

Tutors: Dhabaleswar K. Panda, Hari Subramoni (The Ohio State University)

[More info](#)

SHORTLY

- 01** 11th Open Access Grant Competition results
- 02** Photo gallery from the 6th Annual Conference of IT4Innovations and the 1st Users Conference of IT4Innovations
- 03** Did you visit us on Researchers Night on 6 October, 2017?
See the photo gallery from this event.
- 04** Current vacancies
- 05** Courses offered at IT4Innovations
- 06** Software packages of our colleagues - PermonSVM and PermonQP were published on the PETSc website



THE RESULTS OF THE 11TH OPEN ACCESS GRANT COMPETITION

Throughout June and July 2017, applicants from Czech academic and research institutions applied for a total of 67,845,284 core hours. The Allocation Committee allocated 54,999,384 core hours across 51 successful projects. Most of the computational resources have been allocated to projects in the fields of material sciences (74 %) and biosciences (14 %). The allocated computational resources are available to users from September 2017 to June 2018.

In the 11th Open Access Grant Competition, the computational resources were allocated to a total of 23 different faculties and departments of academic and research institutions. The greatest allocation (33 %) has been awarded to 16 projects of **VŠB – Technical University of Ostrava**, 13 of which are from the university institute IT4Innovations. The projects of the Faculty of Metallurgy and Materials Engineering, Faculty of Civil Engineering, and Faculty of Mechanical Engineering at VŠB-TUO together with IT4Innovations cover all research areas, such as material sciences, biosciences, computer sciences, physics, engineering, Earth sciences, and applied mathematics.

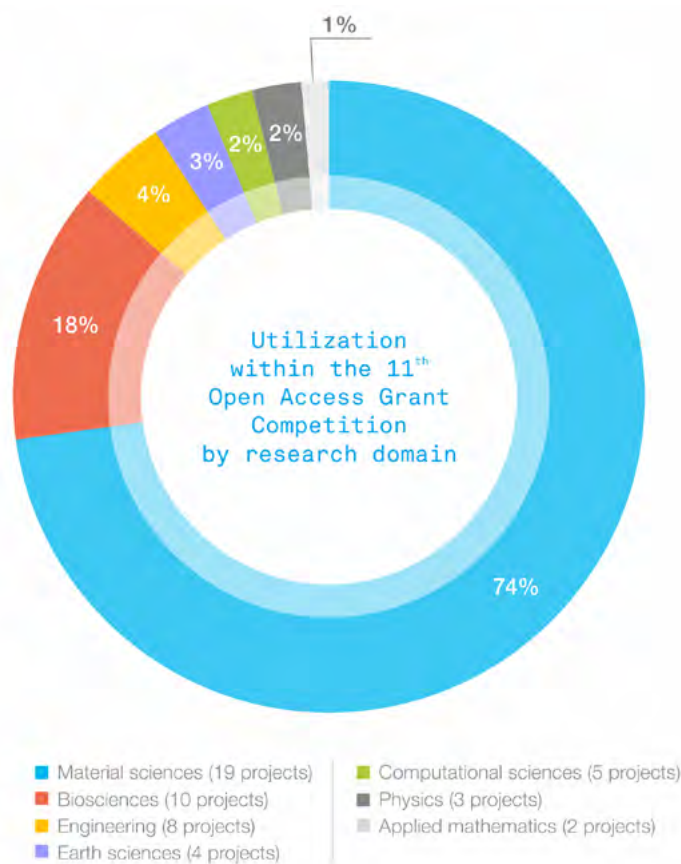
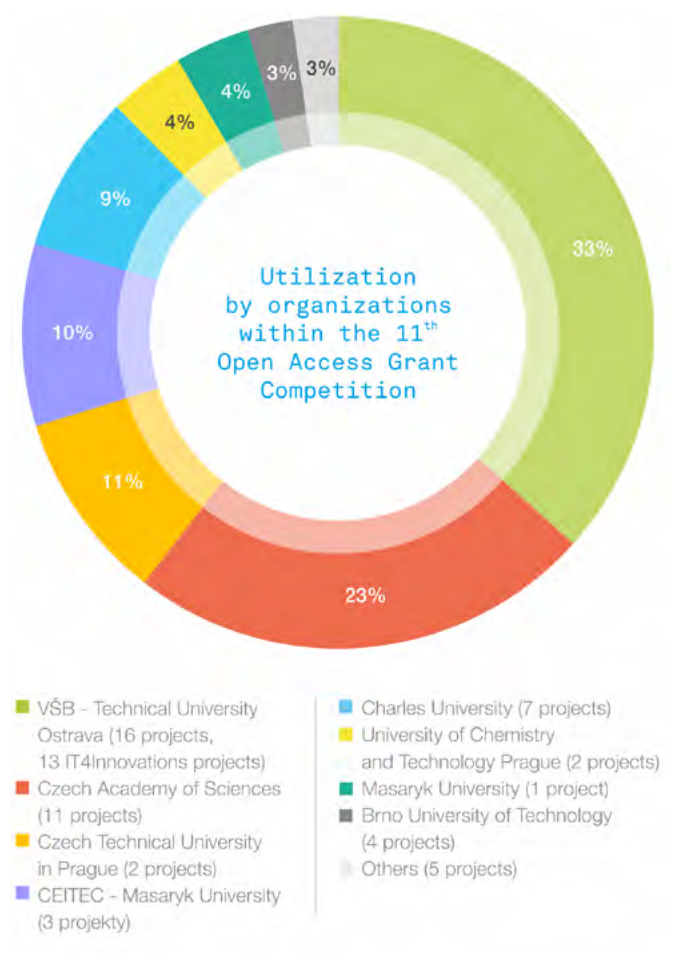
The second largest allocation of computational resources (23 %) has been awarded to 11 projects of the **Czech Academy of Sciences (CAS)**. The CAS research institutes performing their computations using our infrastructure within the 11th Open Access Grant Competition include the J. Heyrovsky Institute of Physical Chemistry, the Institute of Organic Chemistry and Biochemistry, the Institute of Computer Science, the Institute of Atmospheric Physics, the Institute of Plasma Physics, and the Institute of Biophysics. However, most of the projects are from the first two of the above-mentioned institutes. Six of the CAS projects are focused on the field of material sciences.

Other academic and research institutions using our computational resources for their projects within IT4Innovations' 11th Open Access Grant Competition include the Faculty of Electrical Engineering of the **Czech Technical University in Prague**, the Department of Condensed Matter Physics of **Masaryk University** in Brno and the **Central European Institute of Technology** – Masaryk University (CEITEC MU), the Faculty of Mathematics and Physics of **Charles University**, the Faculty of Information Technology of **Brno University of Technology**, and departments of the Faculty of Chemical Engineering of the **University of Chemistry and Technology Prague**.

As in previous Open Access Grant Competitions, the majority of allocated computational resources have been awarded to 19 projects in the field of **material sciences**. In this research domain, the greatest allocation has been awarded to the projects of IT4Innovations (38 %) such as the research of new binary permanent magnets (project of Dr. Dominik Legut) and research of cold rare-gas plasmas which are used in many areas of medicine (project of Ing. Martin Beseda).

A total of 9,045,000 core hours have been allocated to material sciences research projects from Czech Academy of Sciences. For example, at the J. Heyrovsky Institute of Physical Chemistry, density functional theory investigations on properties of zeolite-based catalysts (project of Dr. Štěpán Sklenák) are conducted. One of the projects from the Czech Technical University in Prague is focused on research into nanoscale metallic multilayer composites as novel self-healing materials with extremely low sensitivity to radiation damage (project of Dr. Huseyin Sener Sen).

For the last two years, as is the case with the 11th Open Access Grant Competition as well, the second largest allocation was awarded to **bioscience** projects (14 %). The largest amount of computation time has been allocated to the project of Prof. Pavel Jungwirth from the Institute of Organic Chemistry and Biochemistry of the CAS (2,550,000 core hours) who conducts research on the influence of membrane shape on voltage-gated potassium channels. This research, along with the results of experimental studies, has the potential to provide a better understanding of the synaptic transmission process (transmission of signals between nerve cells).



An introduction to selected projects awarded computational resources within the 11th Open Access Grant Competition

Vojtěch Cima (IT4Innovations): Deep Learning for Novel Drug Discovery

The Deep learning for Novel Drug Discovery project of Ing. Vojtěch Cima has been awarded 400,000 core hours. The allocated computational resources will be used for deep learning in predicting the effects of potential drugs and their possible toxic side effects. Using prediction algorithms, novel drug discovery

and the related costs can simultaneously be accelerated and reduced respectively. This research is carried out as part of the ExCAPE project, the objective of which is to develop algorithms for solving complex pharmacological problems.

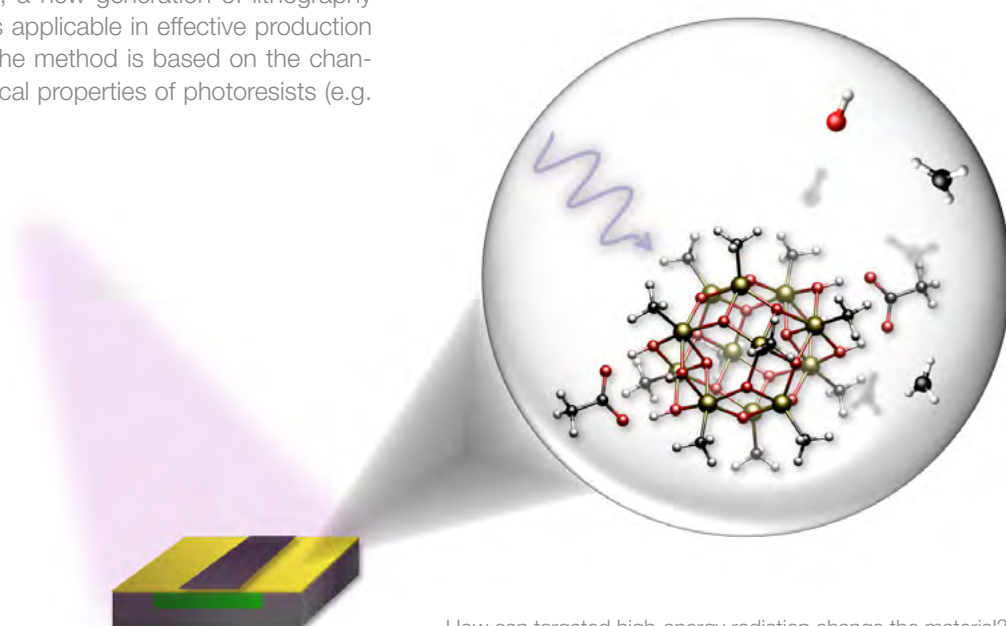
Prof. Petr Slaviček (the University of Chemistry and Technology Prague): Molecular simulations of tin based materials for EUV lithography

How can focused high-energy radiation change a material? What particular changes will occur at a molecular level? The chemical changes of materials under the influence of high-energy photons are studied by the team led by Prof. Petr Slaviček from the Laboratory of the Theoretical Photodynamics Research Group at the University of Chemistry and Technology in Prague. Their project titled Molecular simulations of tin based materials for EUV lithography has been awarded 1,082,000 core hours.

The objective of this project is to describe molecular changes occurring in extreme ultraviolet (EUV) ionization of tin based organic compounds (particularly so-called Sn-O cages). These compounds may potentially be used as photoresist materials for EUV lithography, a new generation of lithography for nanometric dimensions applicable in effective production of new computer chips. The method is based on the changes of physical and chemical properties of photoresists (e.g.

their solubility) after EUV radiation. By exposing specific areas of a material to the radiation, the dimension of the resulting structure can be up to 10 nm, which is the threshold limit dimension of today's commercial chips.

Considerable computational intensity of molecular simulations of ionized Sn-O compounds is generated by the rich electron structure of tin. Simulation of a single trajectory taking half a picosecond requires almost a week to be computed using common processors. With its 76,896 cores (Intel Haswell processors and Intel Xeon Phi accelerators), our Salomon supercomputer will allow the researchers to perform extensive simulation, which would not be practically executable otherwise.

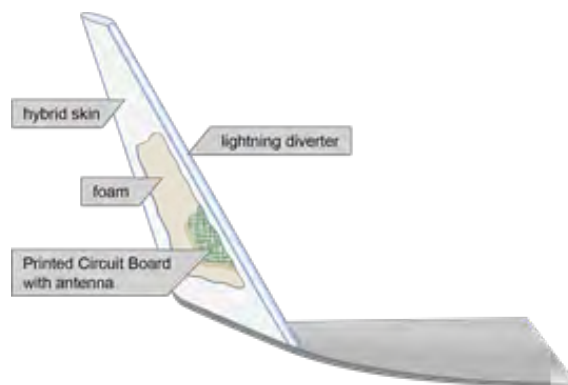


How can targeted high-energy radiation change the material?

Dr. Petr Vrchota (the Czech Aerospace Research Centre): IntA

Design of new regional aircraft and airlines is mainly influenced by economic and environmental factors. Individual parts of airplanes are optimized, for example, with respect to aerodynamic efficiency, fuel consumption, and emissions. Another option for reducing the aerodynamic drag and saving fuel are optimized integrated communication antennas. The antennas usually protrude and contribute to the total drag of the airplane.

The IntA project of Dr. Petr Vrchota from the Czech Aerospace Research Centre has been awarded 200,000 core hours. This project focuses on designing a new winglet with an integrated antenna to improve the flight performance and aerodynamic efficiency of the entire aeroplane and reduce fuel consumption as well as negative environmental impacts. The objective of the research project is to reduce the aerodynamic drag of the aeroplane by up to 2 % using the integrated antenna.



Winglet with an integrated antenna

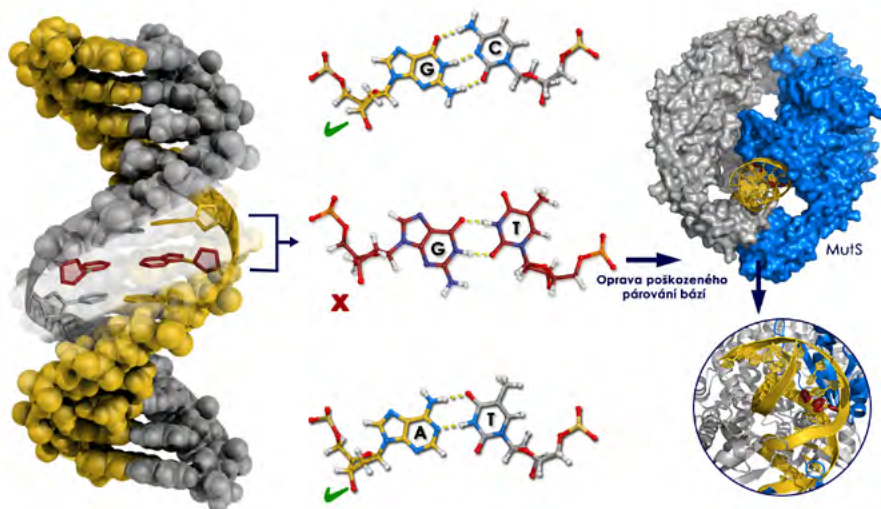
Dr. Petr Kulhánek (CEITEC Masaryk University): Relative Stabilities of Mismatches in Nucleic Acids

The research team led by Dr. Kamila Réblová and Dr. Petr Kulhánek from the Central European Institute of Technology - Masaryk University (CEITEC MU) has been awarded 634,000 core hours for their research into the relative stability of base pairing in deoxyribonucleic acids (DNA).

Chains of the double helix structure of DNA carry genetic information, the integration of which is secured by Watson-Crick complementary pairing. During the process of DNA replication, which occurs when cells divide, this complementarity is used in creating two identical copies of DNA. However, during the replication process, errors such as mismatched base pairs can occur. This is then recognized by various repairation mechanisms. One of them is mismatch repair (MMR), with

the MutS enzyme being the active component in mismatch recognition. When such mismatch is detected, this enzyme activates a cascade of processes leading to its repair.

The allocated computational resources of IT4Innovations supercomputers will allow scientists to perform molecular simulations of short molecules of DNA and focus on describing the stability of all possible combinations of bases containing both the correct Watson-Crick pair and all other combinations. It is believed that this stability can be one of the many factors affecting the effectivity of the MMR mechanism in detecting errors. The information obtained may thus be important for understanding the development of genetically determined diseases or the formation of cancerous growths.



Repair of damaged base pairing



THE 6TH ANNUAL CONFERENCE OF IT4INNOVATIONS AND THE 1ST IT4INNOVATIONS USERS CONFERENCE, AND AN INTERVIEW WITH PAOLO NICOLINI, THE NEW CHAIRMAN OF THE EXECUTIVE BOARD OF THE IT4I USERS COUNCIL

The representatives of the partners of the IT4Innovations Centre of Excellence project, which was implemented in the years 2011 to 2015 within the Research and Development for Innovations Operational Programme, presented the research results and main directions of their research programmes. On the same day, the two-day 1st IT4Innovations Users Conference started. For our colleagues and external users alike, it was an opportunity to present their research projects, for which our supercomputers were used. The invited speakers included researchers from the Czech Academy of Sciences (CAS), Charles University in Prague (CU), and the Czech Technical University in Prague (CTU).

Dr. Michael Komm from the Institute of Plasma Physics of CAS presented the latest news in development of tokamaks and fusion reactors he is involved in. The Institute of Plasma Physics cooperates with the international ITER organization, which initiated construction of an experimental thermonuclear reactor carrying the same name in the south of France in 2007. At

the conference, Dr. Komm presented his research on the computationally demanding PIC simulations of heat flux distribution on plasma-facing components on the walls of the thermonuclear reactor.

Dr. Klára Kalousová from the Faculty of Mathematics and Physics at Charles University seeks to address the question



Awarding PRACE Summer of HPC 2017 Prizes to winners

of whether there is life outside of the Earth. She studies the moons in our Solar System where large amounts of liquid water can be found. At the conference, she presented the results of her research focused on heat transfer and fluid flow in the thick layer of ice on Ganymede, the largest moon of the Solar System.

Dr. Antonio Cammarata from the Advanced Materials Group at the Faculty of Electrical Engineering at CTU in Prague made the participants of the conference familiar with the results of his research focused on materials based on the transition metal dichalcogenides, which can potentially be used as new solid lubricants.

Our colleagues Dr. Lubomír Říha, Dr. Michal Merta, and Ing. Milan Jaroš informed the conference participants of the results and progress in development of the ESPRESO library, BEM4I library, and BLENDER software development, respectively.

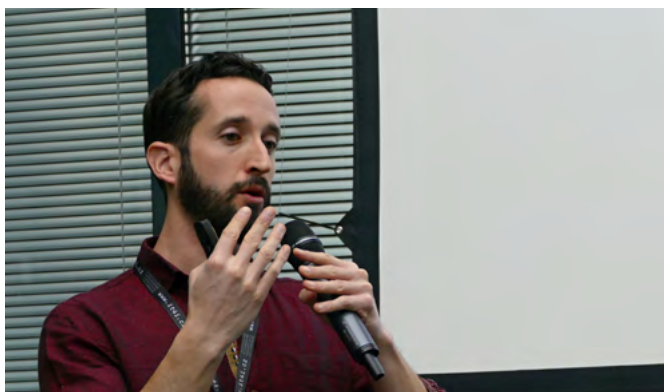
At the conference, the research projects of the external IT4Innovations infrastructure users from the Czech Academy of Sciences, Charles University, the Czech Technical University in Prague, the University of Chemistry and Technology in Prague, the Central European Institute of Technology, Masaryk University, and Brno University of Technology were presented.

At the conference, the 5th PRACE Summer of HPC Award Ceremony took place. The objectives of this Partnership for Advanced Computing in Europe (PRACE) programme include increasing the motivation of students to use high performance computing technologies in their research. This year's winner

of the Best Visualisation Award was Arnau Miro, who worked in the Italian CINECA supercomputing centre on the Web Visualization of the Mediterranean Sea project. The HPC Ambassador Award was won by Mahmoud Elbattah. He proved to be the best HPC promoter with his contributions earning the widest response. At the Aristotle University of Thessaloniki, Greece, he worked on the project Automated Extraction of Metadata from Climate Simulations.

The conference participants were presented with a proposal for establishing the IT4Innovations Users Council (IT4I Users Council, IUC) as the main means of communication between the external users of the IT4Innovations infrastructure and IT4Innovations National Supercomputing Center itself. Dr. Paolo Nicolini from the Czech Technical University in Prague (CTU) was elected as the Chairman of the Executive Board of the Users Council. He works for the Department of Control Engineering at CTU, in the Advanced Materials Group. Paolo Nicolini has been using IT4I infrastructure since the very beginning of the Czech National Supercomputing Center, since 2013, when Anselm was put into operation.

Dr. Nicolini started working at the Department of Control Engineering at CTU, in the Advanced Materials Group lead by Prof. Tomáš Polcar, in June 2013. At that time he was the only non-experimentalist member of the group and, among other things, had to put some effort in locating the computational resources he was going to need. Dr. Nicolini has been using IT4Innovations infrastructure since 2013.



Dr. Antonio Cammarata



Dr. Michael Komm



Dr. Lubomír Říha



Dr. Klára Kalousová

We asked Dr. Nicolini a few questions related to the creation of the IT4I Users Council.

What are your ideas for the newly established IT4I Users Council? What will the Users Council strive to be?

First of all we need to sort out some duties related to the establishment of the IT4I User Council (IUC). This means preparing a document where we state the goals, the composition and other internal rules of the IUC. The Board is currently working on it. Then we can officially start the activities of the IUC. We already have some ideas that we hope could be realized soon. As an example, we would like to set up a platform that will help to strengthen communication between users and the IT4I infrastructure, as well as improve interaction among users themselves. Moreover, I think the IUC will also be involved in discussions about plans for the future of the IT4I infrastructure, providing valuable feedback to the IT4I decision-makers. Then there are other projects that we would like to develop, but I think it is too soon to disclose them now. Stay tuned!

How important do you think it is for your group, and other IT4I infrastructure users, academic and industrial alike, to be part of/involved with the Users Council?

I think it is very important, for different reasons. First of all, as I already mentioned, we will ask all members of the IUC to provide suggestions about the development plan for the IT4I infrastructure. It will be a unique chance for us to stand up and have our voices heard. We also plan to do this for other possible improvements as well. We will try to identify the weak points in the experience of users at IT4I and hopefully contribute to their improvement.

Secondly, but just as important, I see the IUC also as a good opportunity to network between different research groups in the Czech Republic (and abroad). I think that facilitating user interactions will increase the possibility of fruitful collaborations among groups, taking advantage of the different expertise and finally leading to more impactful scientific achievements.

Lastly, I think that IT4I is an excellent HPC center in comparison with other European facilities, providing both top-level computing resources and a qualified and prompt support service. Users should not take this for granted and I think it is wise to put in some effort to maintain the same quality level of the infrastructure or even to try to improve it.

What is your research area, and why does it interest you?

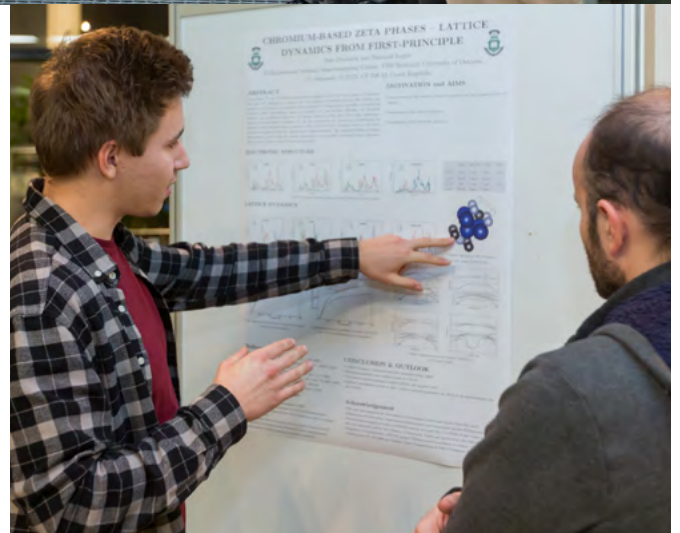
I am a chemist and I work at the border between chemistry, physics and materials science. In my group we study, among other things, friction and lubricants, both from fundamental and applicative aspects. On the one hand we try to identify the mechanisms at work behind the dissipation of energy at the atomistic level, as well as looking for novel materials with improved tribological properties. It is an exciting job (most of the time) because you see the results coming from the simu-



lations that you perform being used by other members of the group (or collaborators) in order to produce real samples that may go quite quickly into people's lives. Moreover, I think as any scientist does, I enjoy tackling open problems, trying to push the border of our knowledge ever further. Some people say that it is more like a passion than a job.

[Can you tell us about the research for which you currently use IT4Innovations infrastructure?](#)

Of course. Currently I am investigating the lubrication mechanism of molybdenum disulfide. This solid lubricant has been known and used for decades, but there are still many unclear points concerning how it works. To gain knowledge about the phenomena that take place in tribological conditions could be critical for finding connections between, for example, the structure of a material and its lubricative properties.



Research poster session

[Thank you for the interview and we look forward to our future cooperation.](#)

Our colleagues at the SC17 booth



PARTICIPATION AT THE SUPERCOMPUTING CONFERENCE SC17 IN DENVER, USA

The Supercomputing Conference (SC) is traditionally held every November. SC is undoubtedly the greatest global meeting of researchers and companies operating in the field of High Performance Computing (HPC). This already 29th Supercomputing Conference took place at the Colorado Convention Center, Denver, Colorado, USA and had almost 13,000 attendees.

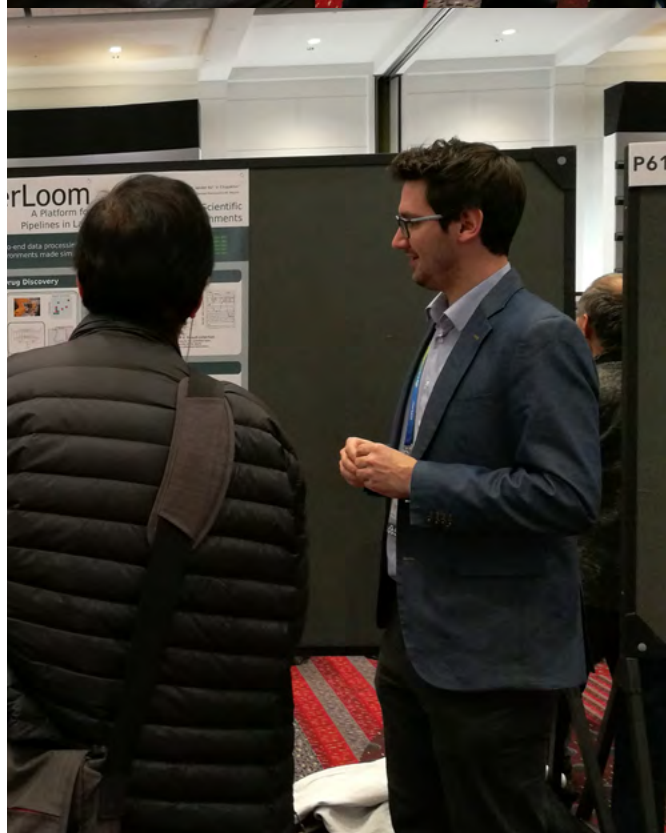
During the six days of the conference, the latest advances in High Performance Computing, artificial intelligence, and machine learning were presented and discussed. An exceptionally exciting and collaborative atmosphere so characteristic of groups of people involved in excellent science using excellent machines prevailed throughout the event. The SC Conference offers a unique opportunity to establish new international contacts, which can open doors for very interesting collaborative research projects.

This SC17 is already the fifth year we have participated as exhibitors. We presented the IT4Innovations infrastructure

and related research of our colleagues in our booth. Visitors were regularly introduced by our colleagues to the **BEM4I** and **ESPRESSO** libraries, **HyperLoom** software, and **HPC as a Service** tool for integrating high performance computing into client applications in order to facilitate user access to massively parallel computers.

In the poster section of the conference, we were represented by our colleagues from the Parallel Algorithms Research Laboratory and Advanced Data Analysis and Simulations Laboratory. Michal Merta and Jan Zapletal, the **BEM4I** library developers, presented their results from using the boundary

Jan Zapletal at the SC17 research poster session

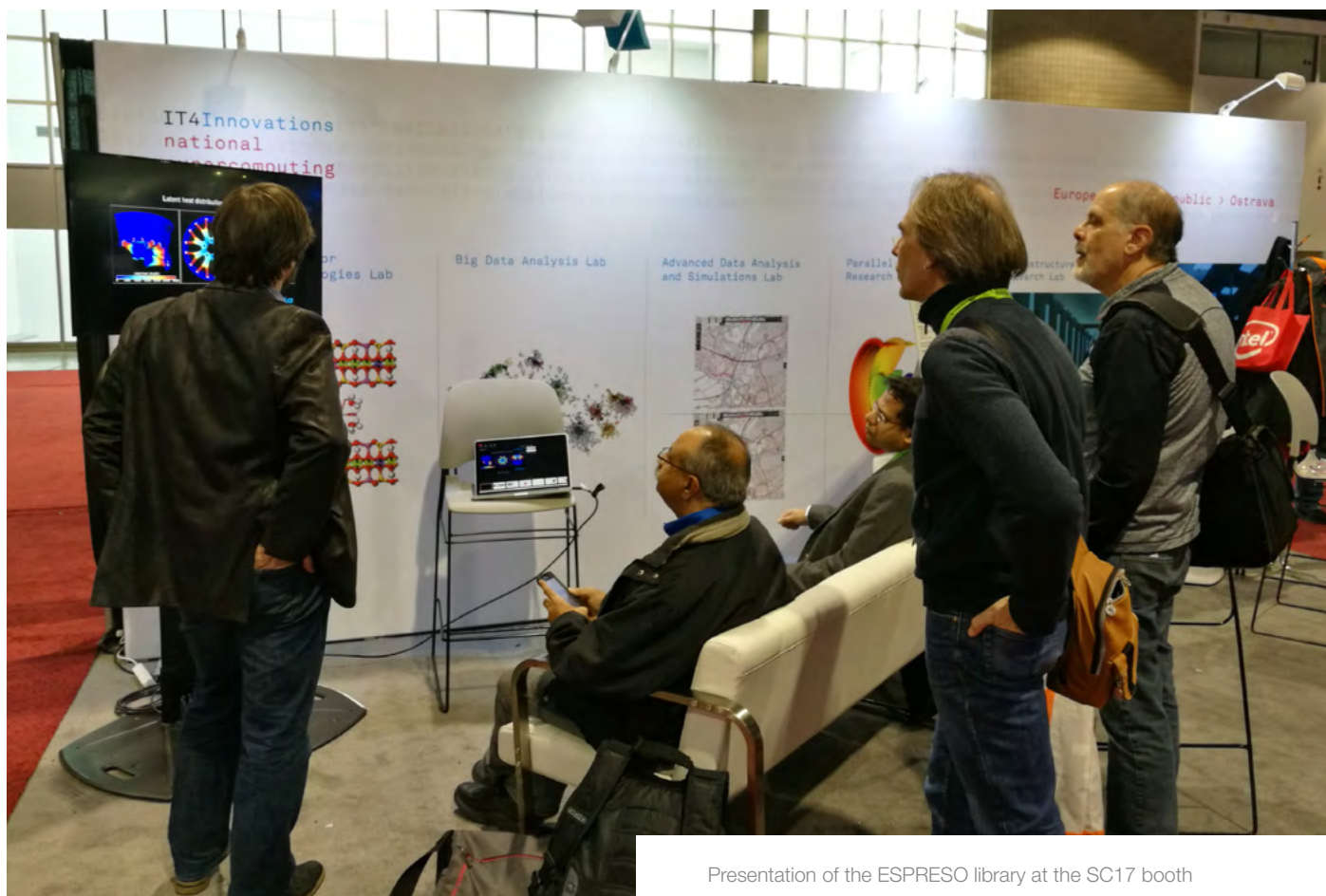


Vojtěch Cima at the SC17 research poster session

element method optimization for modern supercomputing architectures. Vojtěch Cima presented the HyperLoom software for definition and running of complex computing plans containing a large number of interconnected problems, which need to be solved using supercomputers.

Out of the total number of 169 submitted contributions, 98 were accepted for presentation in the poster section. The Technical Programme Committee were so impressed by the poster contributions of our colleagues that they nominated them among the first nine candidates for the Best Poster Award. Even though the nomination was not eventually turned into the prize, the nomination of the two contributions among the nine best posters in the global competition itself is a great success for us. The Best Poster Award was given to the contribution of the University of Tokyo and RIKEN, Japan's largest research institution, titled "AI with Super-Computed Data for Monte Carlo Earthquake Hazard Classification".

Moreover, an updated TOP500 list of the world's most powerful supercomputers was announced at the conference. After two and a half years of operation, Salomon ranking 87th still maintains its position in the TOP100.



Presentation of the ESPRESO library at the SC17 booth

The top 2 positions are occupied by Chinese supercomputers. For one and a half years, the number one position has been maintained by the Sunway TaihuLight supercomputer installed at the National Supercomputing Center in Wuxi, the performance of which is 62 times higher than that of Salomon. Having been in operation for four and a half years, the Tianhe-2 supercomputer installed at the National Supercomputer Center in Guangzhou maintains its number two position. Piz Daint installed at the Swiss National Supercomputing Centre (CSCS) in Lugano, Switzerland, which was upgraded half year ago, maintains the number three position. In the November TOP500 list, the new number four system is Gyoukou installed at Japan's Agency for Marine-Earth Science and Technology. With new accelerators having been installed this year, its performance has increased by 11 times.

The world's fifth most powerful supercomputer is Titan installed at the U.S. Oak Ridge National Laboratory, which was ranked first in 2012. It is worthwhile to mention that our colleagues from the Parallel Algorithms Research Laboratory were also given an opportunity to use the U.S. No.1 supercomputer for their computations. They used Titan for testing and optimization of the massively parallel ESPRESO library, which is also designated for simulations of heat

transfer problems and their optimization. The open-source library was also presented to potential users by its developers at the SC17 conference.

In this November's TOP500 list, both European countries and the USA have each 38 systems ranking in the TOP100. Asia and Australia have 23 and 1, respectively. The European countries with the highest number of supercomputers ranking in the TOP100 include France, Germany, and the UK, each having nine machines. Europe's top 5 most powerful supercomputers are operated in Switzerland, Italy, the UK, Spain, and Germany. Our Polish neighbours operate the Prometheus supercomputer installed at the Academic Computing Centre Cyfronet AGH, which ranks 77th in the TOP500 list. The Czech Salomon is currently ranked Europe's 31st most powerful supercomputer.

In conclusion, 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 the team from the National Supercomputing Center in Wuxi, China, for simulation of the most devastating earthquake affecting China in 1976.



THE STUDENTS OF COMPUTATIONAL SCIENCES DO NOT LET THE GRASS GROW UNDER THEIR FEET, AND DISCOVER THE WORLD THANKS TO THE PRESTIGIOUS SUMMER SCHOOLS

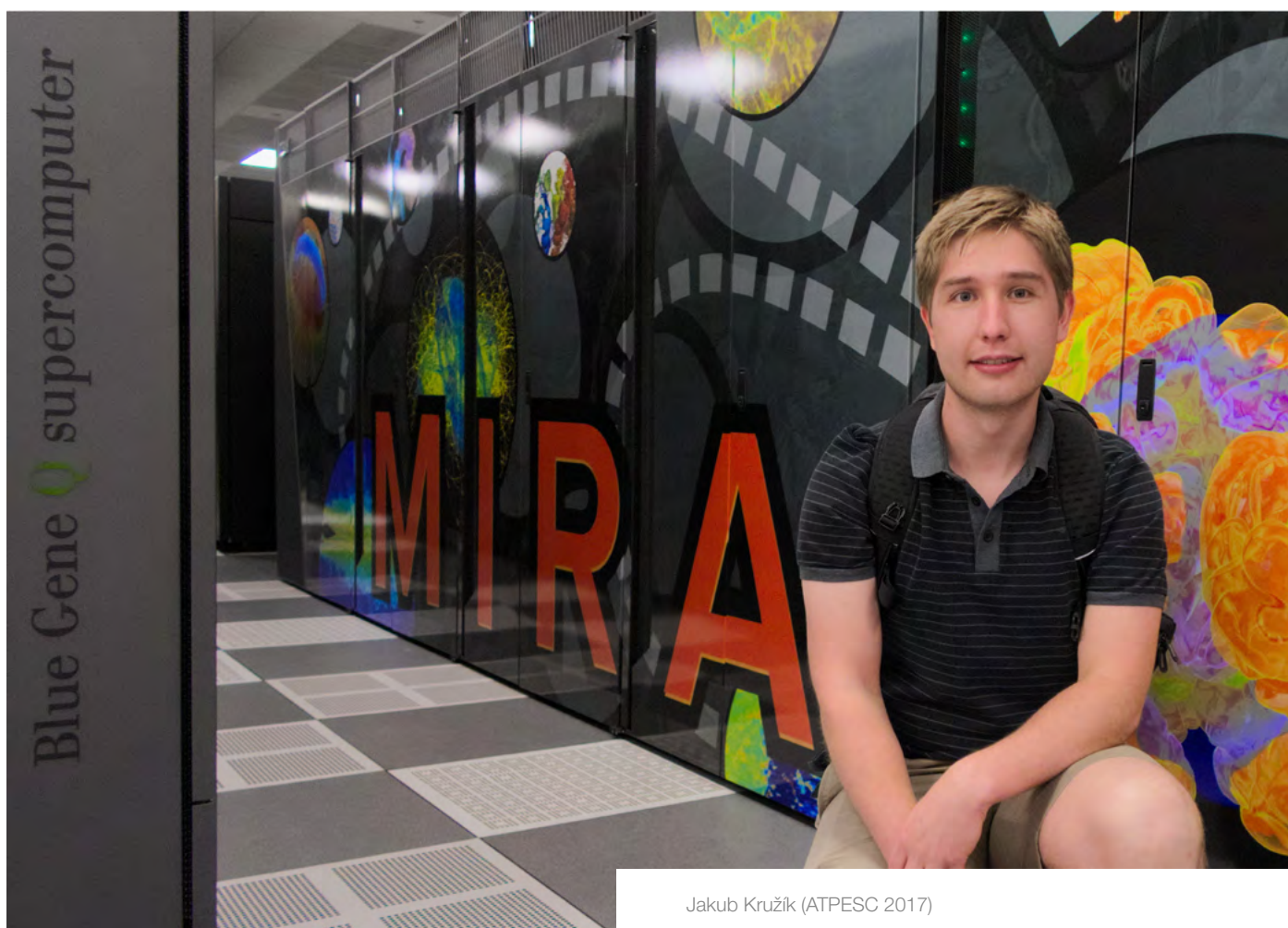
This year, Ondřej Vysocký, Jakub Kružík, Martin Golasowski, and Vít Ptošek participated in three summer training programmes focused on supercomputing. Taking place in the United States of America and Italy, they have all been funded by the organizing institutions

International HPC Summer School on Challenges in Computational Sciences (IHPCSS), Argonne Training Program on Extreme-Scale Computing (ATPESC), and International Summer School on Advanced Computer Architecture and Compilation for High-Performance and Embedded Systems (ACACES).

All students interested in High Performance Computing (HPC) have an opportunity to apply for these summer



Ondřej Vysocký (IHPCSS 2017)



Jakub Kružík (ATPESC 2017)

schools. However, only the best students to be selected by the organizing institution are allowed to participate.

Ondřej Vysocký participated in the week-long International HPC Summer School on Challenges in Computational Sciences (IHPCSS) in Boulder, Colorado, USA, in June 2017. The goal of IHPCSS is to make Computational Sciences students familiar with the use of supercomputers in science worldwide. The costs of the students are covered by the following institutions organizing the training programme: the US-based XSEDE, the pan-European PRACE e-infrastructure, Canadian COMPUTE CANADA, and Japanese RIKEN. In 2018, IT4Innovations is to organize IHPCSS taking place in Prague. The submission of applications was scheduled to start in December. <http://www.ihpcss.org/>

Jakub Kružík participated in the two week-long Argonne Training Programme on Extreme-Scale Computing (ATPESC) in August 2017. This year, ATPESC took place in St. Charles near Chicago, Illinois, USA. The participants go through in-

tensive training in the field of HPC. The summer school is funded by the U. S. Department of Energy, which covers the participants' costs (i.e. accommodation, course fees, etc.). Students interested in ATPESC 2018 can submit their application from December 2017. <http://extremecomputingtraining.anl.gov/>

Martin Golasowski and Vít Ptošek participated in the week-long International Summer School on Advanced Computer Architecture and Compilation for High-Performance and Embedded Systems (ACACES) organized by the European HiPEAC network. This year, it took place in Fiumicino, Italy. ACACES is designed for computer architects and software developers. It is focused on disseminating advanced scientific knowledge and on facilitating international contacts being made between academic institutions and industry. While submitting their application, participants from HiPEAC member institutions can use the opportunity to apply for a grant. The submission of applications is scheduled for the beginning of March. <http://acaces.hipeac.net>

The participants of the prestigious summer schools have answered the following questions:

[What were your initial expectations? What was the purpose of your summer school participation?](#)

Ondřej Vysocký (IHPCSS 2017): My goal was, of course, to attend several interesting lectures. However, the fact that there would be about 80 participating students of a similar age as me from Europe, the USA, Canada, and Japan turned out to be even more attractive as it was a great opportunity to establish many interesting contacts. At the same time, the trans-Atlantic journey was a new, attractive experience for me as well.

Jakub Kružík (ATPESC 2017): My goal was to not only extend my existing knowledge but also acquire new knowledge necessary for efficient use of today's, as well as future state-of-the-art supercomputers.

[What was the programme of this year's summer schools and what were the most interesting things you learned?](#)

Ondřej Vysocký (IHPCSS 2017): The event consisted of many lectures focused on the fundamentals of parallel programming as well as on software development. Due to two parallel sections, there was sufficient information available for students who are not primarily focused on programming, yet at the same time, it was possible to choose more advanced topics as well.

The first days would not do without the typical poster sections, where all students, one after another, presented their research (divided in alphabetical order into 4 groups so that it was possible to see the posters of others as well). The composition of the participants based in many different scientific domains made this section very interesting.

A significant amount of time was dedicated to mentoring, with the organizers sharing their experience in order to help students get a much clearer idea about working in the HPC field and in doctoral studies in general. I personally consider this part beneficial primarily for master students thinking about their future career in research.

Jakub Kružík (ATPESC 2017): The most interesting topics for me included numerical algorithms and software, hardware architectures, and programming models and languages. Apart from the lectures, we also had a chance to test our newly acquired knowledge during the practical sessions. In addition, we had access to the largest supercomputers (e.g. Titan, Cori, Mira, Theta) located in the supercomputing centres under the U. S. Department of Energy Office of Science. The programme is unique with its wide scope and selection of lecturers, who are world-class leaders in the field of HPC. The lecturers in the numerical algorithms section included, among others, J. Demmel, B. Smith, J. Dongarra, and D. Keyes. The

lectures were often led by the main authors of the given software or model. Thus, for example, the lectures on advanced functions of MPI were led P. Balaji, B. Gropp, and R. Thakur – all are among the members of the MPI Forum, which creates the MPI standard.

Vít Ptošek (ACACES 2017): It consisted of a set of pre-selected courses according to the preferences. Each participant could choose 4 out of 12 courses, which were then divided into three to four blocks for each day. The primary focus was on HPC and clouds, but one could choose quantum computing as well (which I did).

[What have you gained from participating in the summer school?](#)

Ondřej Vysocký (IHPCSS 2017): I would say that participating in this programme I have gained exactly what I expected to gain from it, and getting a lot of new contacts, in particular, is invaluable. Unfortunately, I have not managed to use the newly acquired technical knowledge yet, which will surely change in the future. IHPCSS was perfectly organized with a portfolio of high-quality lectures and interesting people.

Jakub Kružík (ATPESC 2017): I have gained information about where the current trend of supercomputers and the way their efficient utilization are heading. I have also learned about new methods and programming models. Additionally, I have established many new contacts with both the lecturers and participants. The course is great quality and what is more, it is free of charge. I certainly recommend it.

Vít Ptošek (ACACES 2017): Apart from a lot of information from the highly-qualified lecturers, I have gained plenty of new contacts established through networking. I have acquired entirely new knowledge and deepened the existing one. Moreover, I was offered a grant fully covering all but the travel costs.

[Would you recommend participation in this summer school to other students?](#)

Ondřej Vysocký (IHPCSS 2017): IHPCSS containing plenty of top lectures and interesting people was perfectly organized. If somebody decided to participate next year, they would save a lot of money on travelling, as the following summer school co-organized by IT4Innovations will take place in Prague.

Jakub Kružík (ATPESC 2017): The course is high quality and what is more, it is for free. I would surely recommend it.

Vít Ptošek (ACACES 2017): In any event, ACACES is a high-quality summer school focused primarily on high performance computing, and it appeals to both HW and SW solution advocates. It all takes place in a pleasant environment, and I am sure that this school is beneficial for students, professionals, and lecturers. In my opinion, it was all very well organized.

ESPRESO FEM HEAT TRANSFER MODULE

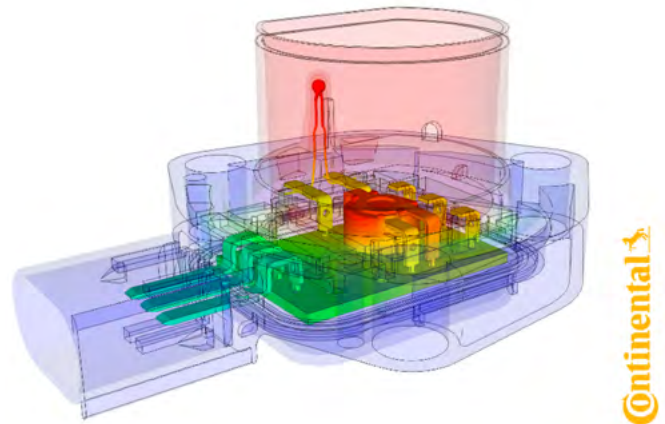
Highly parallel finite element package
for engineering applications

The latest technological advances in computing have brought a significant change in the concept of new product design, production control, and autonomous systems. In the last few years, we have been witnessing considerable transition to virtual prototyping and gradual pressure on integrating large parts of the industrial sector into the fourth industrial revolution (Industry 4.0).

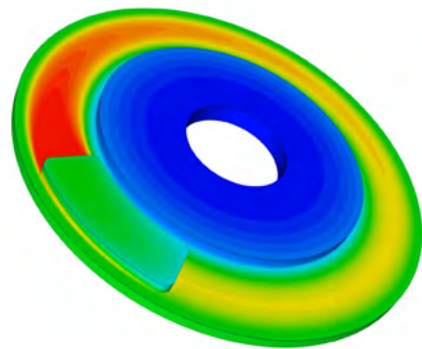
The main objective of the ESPRESO library development team is to create a complete open-source package applicable to a wide range of complex engineering simulations in areas such as mechanical engineering, civil engineering, and the energy industry. The free licence for the developed package allows automatized simulation toolchains such as systems for shape optimization to be created above the ESPRESO library. The added value of this package is a highly scalable solver based on the methods of domain decomposition, which allows the computational capacity of state-of-the-art supercomputers to be fully utilized, and thus solve problems with billions of unknowns. In addition, the advantage of this package is also its simple interface for configuration of the implemented solvers. Development of a heat transfer module for engineering applications, within IT4Innovations projects, has just been finished by the development team. The researchers use this tool for implementing contract research projects, and its further development is supported through participation in several European projects. The ESPRESO FEM Heat Transfer Module has been used, for example, in response surface evaluation with several design variables in thermal sensors, in cooperation with Continental.

Prospective future connection to both cloud centres within the H2020 CloudiFacturing project and HPC as a Service developed by our colleagues will facilitate the use of modern technologies by external partners primarily from small and medium enterprises in the context of virtual prototyping.

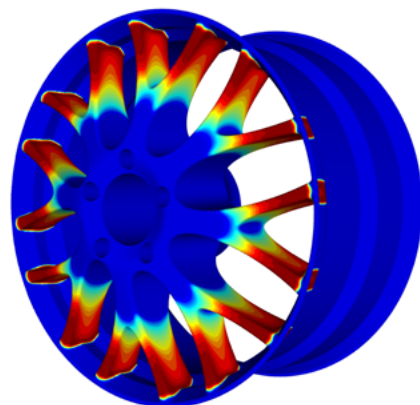
In the upcoming year, the ESPRESO FEM development team will be involved in developing a module for topological optimization and integration of non-linear domain decompositions for accelerating non-linear computations.



Cooperation with the Continental Company in designing the thermal sensor



Transient simulation of the disc brake



Latent heat distribution under the solidification of the aluminium



PARTNERSHIP WITH BAYNCORE

On the 1st of November 2017 IT4Innovations initiated a partnership with Bayncore (United Kingdom).



Its first project includes contracted research and consultancy services to Bayncore as part of the Intel AI EMEA Roadshow. More specifically, it includes the creation of Machine Learning related content, and co-conducting training sessions throughout the EMEA region (Europe, Middle East and Africa) in strong collaboration with Bayncore and Intel. Some of the topics covered are code modernization using Intel Software Development Tools, Intel optimized Deep Neural Networks and Machine Learning with Tensorflow, Caffe and scikit-learn, and the Intel Python Distribution.

IT4Innovations' Advanced Data Analysis and Simulations Laboratory members Jan Martinovič, Georg Zitzlsberger, Vojtěch Cima and Martin Golasowski are involved in this initial partnership with Bayncore.

The first contributions have already been made to events in Oxford, Madrid and Paris in early November. Other events took place in Johannesburg/Pretoria and Tel Aviv in December. More events are scheduled for the beginning of 2018.

Bayncore website:

www.bayncore.com

Intel AI EMEA Roadshow:

www.intel.co.uk/content/www/uk/en/events/ai-emea-roadshow

About Bayncore:

Bayncore Limited is a Consulting and IT services firm specialised in providing a platform of high tech solutions for HPC, Technical Computing and Big Data. Bayncore is based in London and Cambridge in the United Kingdom, and is covering the EMEA territories.

Bayncore's offers, mostly tailor-made for each client, are structured around 4 lines of services:

- A Platform of High Tech IT Services & Consulting
- Training
- Benchmarking
- Research & Development

Bayncore is a Partner of:

- Intel
- Microsoft
- Polyhedron Software
- Computer Laboratory – University of Cambridge (UK)