IT4Innovations national supercomputing center

NEWSLETTER

Q2 2017

Results of the 10th Open Access Grant Competition

The 10th Open Access Grant Competition and its results were announced at the end of January 2017, and in May 2017, respectively. The applicants requested 78,757,000 core hours in total. 55,555,000 core hours have been allocated among 50 successful applicants. As in the previous Open Access Grant Competition, most of the computational resources, 80 % of all the computational resources allocated within this call, have been allocated to projects in the field of material sciences and biosciences.

Read more

IT4Innovations infrastructure upgrade

The new successfully approved IT4Innovations National Supercomputing Center – Path to Exascale project will enable upgrading of our supercomputing infrastructure as well as supporting relevant research.

Read more

Example of successful research of our users

The international DATE 2017 conference prize for the best interactive presentation has been awarded to our users from Brno University of Technology.

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About the conference High Performance Computing in Science and Engineering 2017

An interview with Radek Tezaur, one of the invited speakers

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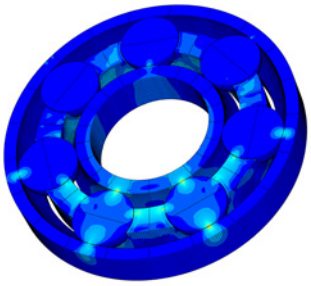
NEWSLETTER Q2 2017

Report from the International Supercomputing Conference, TOP500 list update

The list of the fastest supercomputers in the world „TOP500“ was updated in June 2017. Has the list changed much?

Read more



TETRAMAX and CloudiFacturing, new international projects we will join

Two new projects have been approved for funding under EU Horizon 2020.

Read more

IT4Innovations has become a PRACE training centre

A portfolio of our own courses for PRACE, which is planned for the academic year 2017-2018

Read more

Jan Zapletal has been awarded the Joseph Fourier Prize for computational sciences

Our colleague has won first place in the nationwide Joseph Fourier Prize competition for the best research within PhD studies in the field of computational sciences.

Read more

11th Open Access Grant Competition

Apply for the computational resources of our supercomputers within the 11th Open Access Grant Competition. Applications can be sent until **July 27, 2017**. 48,000,000 core hours are to be distributed. The period to use allocated computational time is expected to start on **September 22, 2017 and end on June 19, 2018.**

More information

INVITATIONS

Researchers' night

Come to IT4Innovations on **Friday October 6, 2017 at 5pm**, and have a look at the most powerful Czech supercomputer Salomon. You will have the opportunity to meet researchers and become a researcher for the night! The main theme of Researchers' night 2017 is mobility. See the photos from last year's **Researchers' night** and do not miss out on this unique event this year. Add the date to your diary, **October 6, 2017**, and come to visit us. We look forward to seeing you.

SHORTLY

01 Publication Review 2016

02 Photo gallery from the conference High Performance Computing in Science and Engineering 2017

03 We are looking for new collegues for the Supercomputing Center team

RESULTS OF THE 10TH OPEN ACCESS GRANT COMPETITION

The 10th Open Access Grant Competition and its results were announced at the end of January 2017, and in May 2017, respectively. The applicants requested 78,757,000 core hours in total. 55,555,000 core hours have been allocated among 50 successful projects.

As in the previous Open Access Grant Competition, most of the computational resources totalling 44,495,000 core hours have been allocated to projects in the field of material sciences and biosciences, which is 80 % of all the computational resources allocated within this call.

The first three largest allocations come under the field of material sciences. The largest allocation, totalling 11,069,000 core hours, has been awarded to the research of our colleague Dr. Dominik Legut in the area of novel superconductors. Prof. Pavel Hobza from the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences (CAS) has been awarded the second largest allocation, totalling 7,420,000 core hours, for in silico drug design. The third largest allocation, totalling 5,187,000 core hours, has been awarded to the project of Prof. Mojmír Šob from the Central European Institute of Technology, CEITEC MU, Masaryk University in Brno, who conducts research in superalloys.

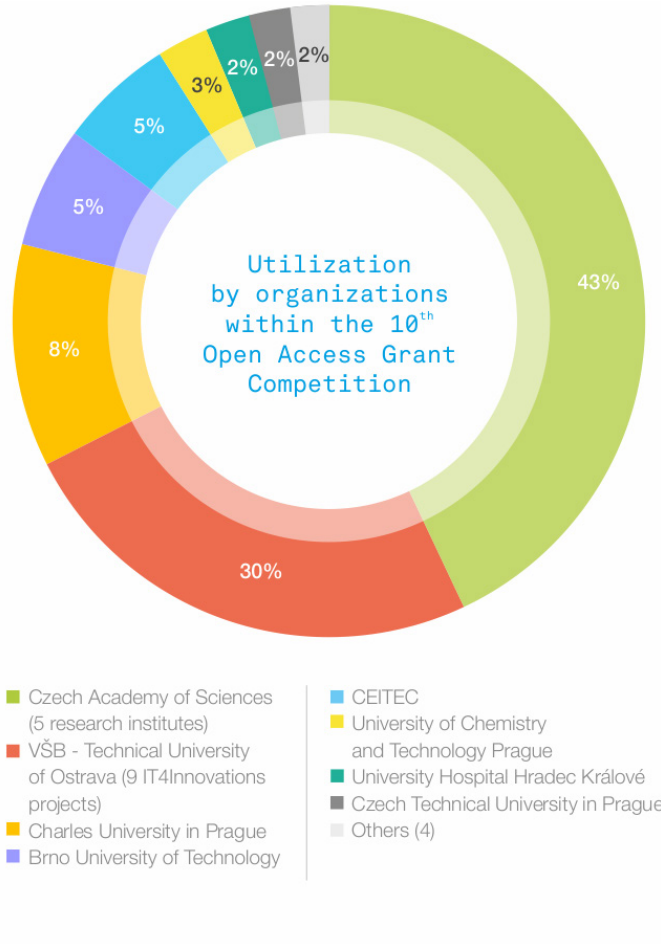
The three largest allocations in the field of biosciences have been awarded to the projects of the following scientists. Dr. Lubomír Rulíšek from the Institute of Organic Chemistry and Biochemistry of the CAS has been awarded 3,150,000 core hours for his computational biochemistry research,

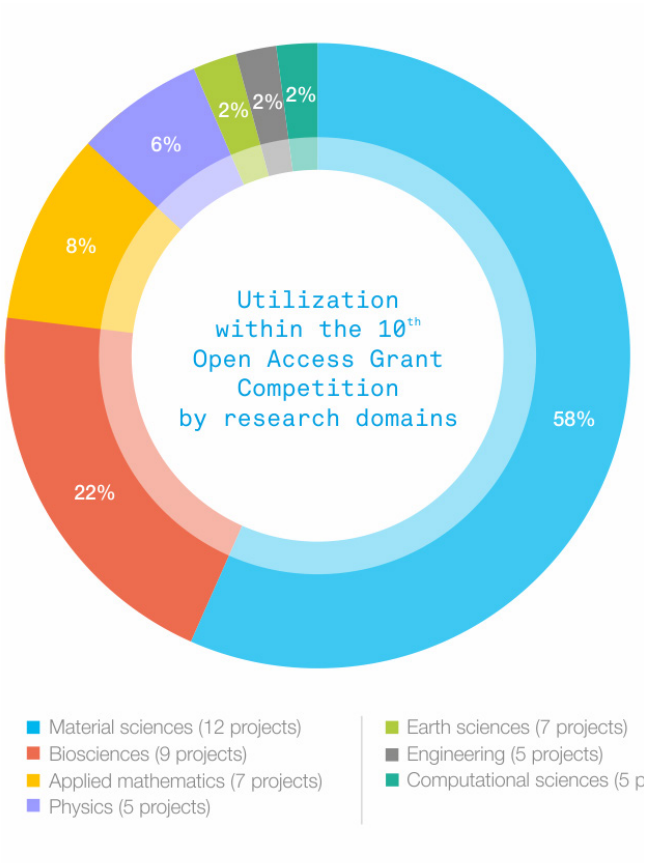
particularly protein structures. Mgr. Ondrej Gutten, also from the Institute of Organic Chemistry and Biochemistry of the CAS, has been awarded 1,730,000 core hours for his research in metal-protein interactions. The project of Dr. Jiří Jaroš from Brno University of Technology has been allocated 2,678,000 core hours for validation of computational models of ultrasound propagation in biological tissues.

Across the other fields of research, the computing time has been awarded to seven projects in the field of applied mathematics (including 3 projects of IT4Innovation's in-house applicants) and seven projects focused on Earth sciences research (including 5 projects of applicants from Charles University). Computing time totalling 5,383,000 core hours has also been allocated to 15 projects in the field of physics (including 3 projects of the CAS), engineering (e.g. the project of the National Center for Research, Development and Testing in Aerospace), and informatics (including two projects of Brno University of Technology).

The largest part of the computational resources has been allocated to the Czech Academy of Sciences. Eleven projects have been awarded 23,564,000 core hours, which is nearly 43 % of the total allocated computing time. The CAS research institutions, which perform their computations within our 10th Open Access Competition, include the Institute of Organic Chemistry and Biochemistry, the Global Change Research Institute, the Institute of Physics, the J. Heyrovský Institute of Physical Chemistry, and the Institute of Plasma Physics. The CAS projects are mainly focused on the fields of biosciences, material sciences, and physics.

A total of 12 projects from VŠB – Technical University of Ostrava, mainly from IT4Innovations, have been awarded 16,638,000 core hours, which is 30 % of the total allocated computing time. The projects are mainly focused on the fields of applied mathematics, material sciences, and computational sciences. Ten projects from Charles University have altogether been awarded 4,586,000 core hours, with half of the projects being focused on Earth sciences.

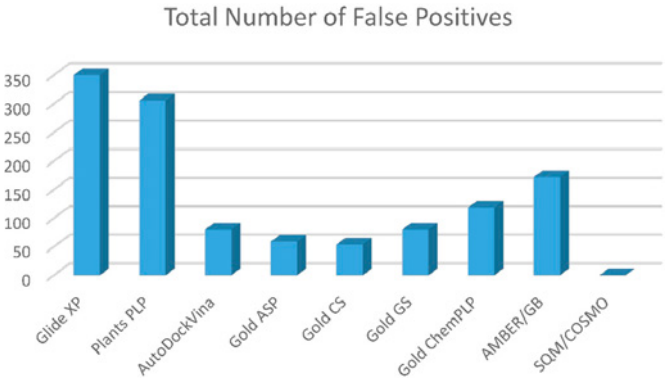




A selection of the projects awarded computational resources within the 10th Open Access Grant Competition

Prof. Ing. Pavel Hobza, DrSc., FRSC
(Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences): In silico drug design

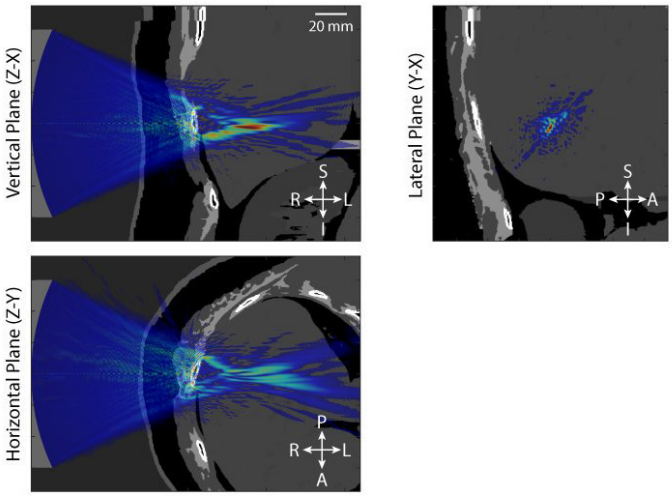
Prof. Pavel Hobza from the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences conducts research on computer-aided drug design. His project "In silico drug design" has been awarded 7,425,000 core hours within the 10th Open Access Competition. The allocated computational resources will be used for developing virtual screening methods for drugs. Used by the pharmaceutical industry, this approach is based on molecular modelling (docking and scoring) in order to identify suitable substances for designing new drugs. Due to its high computing performance requirements, the reliability of these methods has been low so far. Using the IT4Innovations supercomputers and employing exact quantum chemistry computations, the researchers from Prof. Hobza's team are able to predict both the drug structure at the active site of proteins and their ability to bind, which determines their therapeutic effects. The recently published approach is currently used in collaboration with leading pharmaceutical companies.



Number of false positive results for various protein-ligand complexes for both the used scoring functions as well as the newly designed function based on quantum chemistry computations (SQM/COSMO)

Dr. Ing. Jiří Jaroš (Brno University of Technology):
Experimental verification of computer simulation of non-linear ultrasound propagation through biological tissues

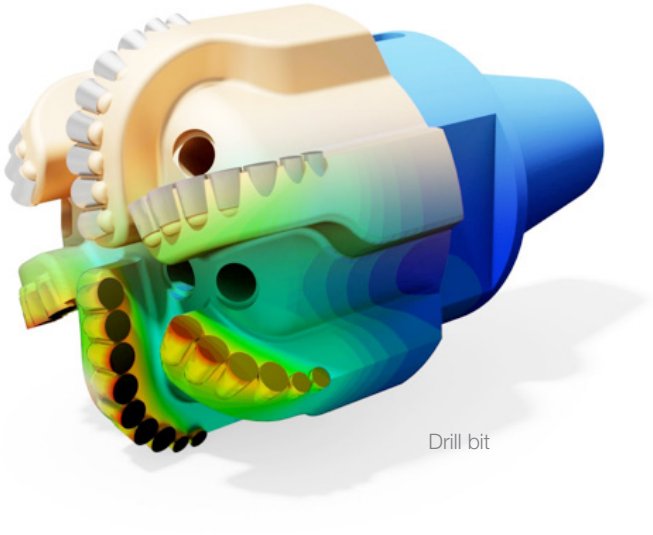
The research team of Dr. Jiří Jaroš has been awarded 2,678,000 core hours for their research in the field of computer simulations of ultrasound propagation in biological tissues. The researchers focus on targeted ultrasound, which is applied in the treatment of non-invasive cancer and other diseases. The targeted ultrasound is based on the principle of focusing high-power ultrasound beams through biological tissues. Surgeons are thus able to remove a tumour from the body of their patients using a non-invasive procedure.
The results of the ultrasound surgery, however, are influenced by many factors, such as presence of bones, large blood vessels, and fat surrounding organs. These factors lead to attenuation, scattering, and reflection of the ultrasound wave, which then does not have enough energy in the required area. Therefore, the awarded allocation will be used by the research team from Brno University of Technology for evaluating the accuracy and optimization of the models of ultrasound propagation in biological tissues.



Sonication in the liver with strong rib distortion

Dr. Ing. Tomáš Brzobohatý (IT4Innovations):
ESPRESO FEM – Heat Transfer Module

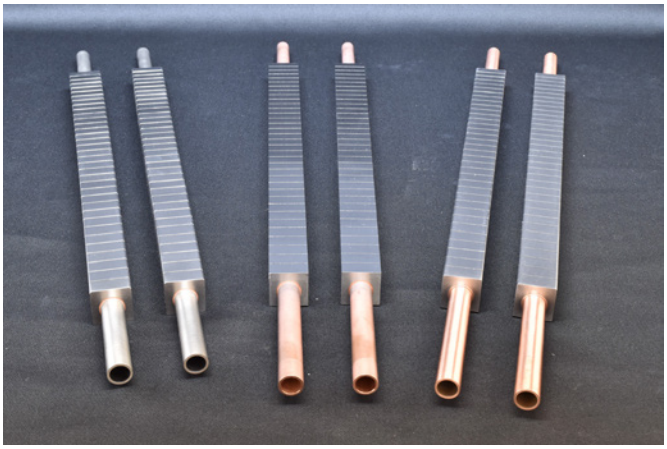
The project by Dr. Tomáš Brzobohatý "ESPRESO FEM – Heat Transfer Module" has been awarded 2,425,000 core hours. The research team will focus on developing and testing the finite element method-based complex and massively parallel library for performing simulations of heat transfer problems, and their optimization. This library includes the massively parallel iterative ESPRESO solver continually developed at IT4Innovations.



Drill bit

Dr. Mgr. Michael Komm (Institute of Plasma Physics of the Czech Academy of Sciences):
PIC simulation of heat flux distribution on plasma-facing components in thermonuclear reactor components and experiments in the WEST tokamak

Researchers from the Institute of Plasma Physics of the Czech Academy of Sciences are involved in the research associated with a long-term international effort to tame thermonuclear fusion. The project of Dr. Michael Komm has been awarded 300,000 core hours, and focuses on modelling the deposition of heat transferred by plasma particles on the plasma-facing components. The research focuses on the experiments in the WEST tokamak, located in Cadarache in Southern France, where the prototypes of the components designated for the currently built ITER tokamak will be tested. As the first fusion device, ITER is supposed to generate more energy than it consumes. However, this is linked with extreme heat fluxes reaching the material limits of the plasma-facing components. The objective of the Czech Academy of Sciences project is to find out whether the understanding of the interaction of plasma and the plasma-facing components is accurate enough for successful operation of the thermonuclear reactor.

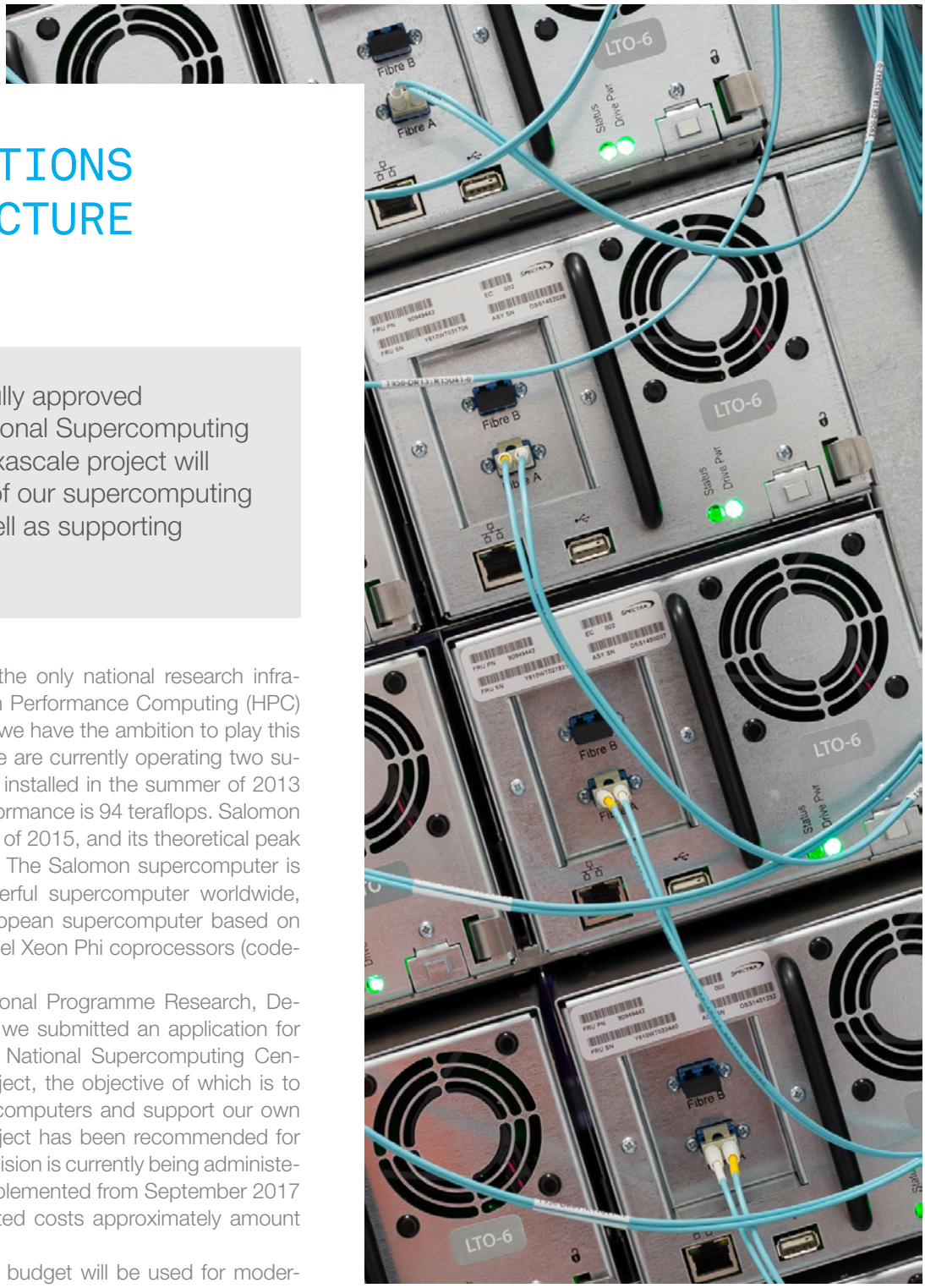


Prototypes of the actively cooled diverter components for the ITER Tokamak that will be tested in the WEST Tokamak

10th Open Access Competition results available here:
http://www.it4i.cz/computing-resources-allocation/10th-open-access-competition-results/?lang=en

IT4INNOVATIONS INFRASTRUCTURE UPGRADE

The new successfully approved IT4Innovations National Supercomputing Center – Path to Exascale project will enable upgrading of our supercomputing infrastructure as well as supporting relevant research.



IT4Innovations is currently the only national research infrastructure in the field of High Performance Computing (HPC) in the Czech Republic, and we have the ambition to play this role in the future as well. We are currently operating two supercomputers. Anselm was installed in the summer of 2013 and its theoretical peak performance is 94 teraflops. Salomon was installed in the summer of 2015, and its theoretical peak performance is 2 petaflops. The Salomon supercomputer is ranked the 78th most powerful supercomputer worldwide, and the most powerful European supercomputer based on the first generation of the Intel Xeon Phi coprocessors (code-named Knights Corner).

In 2016, within the Operational Programme Research, Development, and Education, we submitted an application for funding for "IT4Innovations National Supercomputing Center – Path to Exascale" project, the objective of which is to upgrade the existing supercomputers and support our own research. This year, the project has been recommended for funding, and the funding decision is currently being administered. The project is to be implemented from September 2017 to August 2021. Its estimated costs approximately amount to 503,031,000 CZK.

Almost 80 % of the project budget will be used for modernization and upgrade of the existing Anselm and Salomon systems. The systems will be upgraded in order to keep up with other developed countries on their path towards exascale supercomputers, which are up to a thousand times more powerful than the current systems.

Along with this project, the research led by Prof. Dr. Ing. Jaromír Pištora, Dr. Ing. Dominik Legut, and Dr. Mgr. Pavel Tomančák in the field of modelling photonic and spinphotonic structures, novel progressive material design based on the electronic structure calculation, and bioimage analysis using HPC, respectively, will also be supported. These fields are very progressive and require upgraded computing capacity. Simulation and HPC are currently significant tools in research and their importance will continue to increase in the upcoming years.

Best interactive presentation award at the conference Design, Automation and Test in Europe, DATE 2017

EXAMPLE OF SUCCESSFUL RESEARCH OF OUR USERS

The international DATE 2017 conference prize for the best interactive presentation has been awarded to our users from Brno University of Technology.

Prof. Dr. Ing. Lukáš Sekanina, Doc. Dr. Ing. Zdeněk Vašíček, Ing. Radek Hrbáček, and Ing. Vojtěch Mrázek from the Evolvable Hardware research group (Faculty of Information Technology at Brno University of Technology) have received a prize from the international Design, Automation and Test in Europe 2017 conference for the best interactive presentation.
The DATE conference is one of the largest and most prestigious events focused on automation of computer systems design worldwide. At the DATE 2017 conference held in March 2017 in Lausanne (Switzerland), the interactive presentation of our users from Brno University of Technology was awarded the above-mentioned prize in a highly competitive environment comprised of 90 other interactive presentations. The contribution of our users entitled „EvoApprox8b: Library of Approximate Adders and Multipliers for Circuit Design and Benchmarking of Approximation Methods“ presented a new library of approximate adders and multipliers, which can be applied in low-input circuit architectures, such as neural networks on chips, and the Internet of Things. An interesting feature is that the library has been automatically generated by means of artificial intelligence methods – using parallel evolutionary algorithms. On our supercomputers, they have implemented their own evolutionary design, requiring massive computing power.

Project website: http://www.fit.vutbr.cz/research/groups/ehw/approxlib/index.html

THE HIGH PERFORMANCE COMPUTING IN SCIENCE AND ENGINEERING 2017 CONFERENCE

The 3rd High Performance Computing in Science and Engineering conference took place between 22nd and 25th May 2017, at the Hotel Soláň in the Beskydy mountains. The objectives of the conference were to exchange knowledge and present current research results in the field of applied mathematics, numerical linear algebra, optimization methods, computational sciences, and high performance computing.

The High Performance Computing in Science and Engineering 2017 conference was attended by almost 100 experts and students. Some of the speakers travelled from far afield. The conference hosted participants from the United States of America, including Yousef Saad (University of Minnesota), Ludmil Zikatanov (Pennsylvania State University), Erin Claire Carson (New York University), and Radek Tezaur (Stanford University).

There was also a scientific poster presentation session within the conference programme. From a total of 24 posters, the best poster, as voted for by conference participants, was entitled 'PERMON', and was made by our colleagues Doc. David Horák, Dr. Martin Čermák, Dr. Václav Hapla, Ing. Marek Pecha, Ing. Radim Sojka, Ing. Jiří Tomčala, and Bc. Jan Kružík.

INTERVIEW WITH RADEK TEZAUR, ONE OF THE INVITED SPEAKERS

At the conference venue, we used the opportunity to ask Radek Tezaur, one of the invited speakers, a few questions. Radek Tezaur completed his PhD in Applied Mathematics at the University of Colorado in Denver (USA), and he is currently working at Stanford University in California.

Your studies and career are filled with mathematics. Can you remember the moment when mathematics captivated you so much that you decided to pursue it in your studies and career alike?

I cannot really say that mathematics has become my fate one particular day. My interest in it has emerged gradually. First, I was captivated by its formal structure, a certain level of playfulness it allows, and in the end, it was mainly for its ability to represent physical processes. In fact, for this particular reason, I had originally studied theoretical physics at the Faculty of Mathematics and Physics at Charles University in Prague before I moved into mathematical modelling, led by Prof. Nečas.

After completing your studies at Charles University in Prague, you found yourself in Colorado (USA). There you studied for a PhD in applied mathematics for five years at the University of Colorado. Was there anything surprising for you at the beginning of your PhD studies?

Since it was a relatively short time after the Velvet Revolution and it was my first time in the USA, everything was kind of new for me. With respect to the study itself, I was surprised by the informal relationship between professors and students as well as the flexibility in choosing lectures. For sure, I appreciated the good fundamental knowledge I acquired at the Faculty of Mathematics and Physics. However, I have to say that I did not learn some of the more advanced concepts in such standard subjects such as linear algebra until my stay in Colorado. Apart from my studies there, particularly pleasant surprises were the friendly and smiling people of Colorado, as well as the ease with which I could manage the matters of daily life.

You are currently working at Stanford University in California. This university is the birthplace of some breakthrough technological innovations such as Google, Cisco, and Yahoo! Can you describe the environment of this university to us?

Stanford was founded as a practical (applied) counterpart to the East Coast elite universities, and as such it remains faithful to its legacy. The university has long been taking advantage of its location in Silicon Valley, and it is undoubtedly vice versa as well. Hardly a day goes by without a story of a student or professor who left Stanford only to found a company worth a million-dollars. I still find myself being surprised by the quality of the students. At the same time, it is not always easy to keep them here for PhD studies since they are highly sought after in the Silicon Valley or anywhere else.

What does your usual working day look like?

My working day starts after tackling the traffic in Silicon Valley. I spend most of my working time on our projects, our software development, and working with students. I meet them regularly in order to learn about their progress. My door is always open to them. They can pop into my office and discuss solutions to current problems.

We are talking at the HPCSE conference venue organized by IT4Innovations in your homeland. At the HPCSE 2017 conference, you have presented the research of your research group in the Aeronautics and Astronautics Department at Stanford University focused on "Reduced order models for direct and inverse acoustic problems". Can you please make those who could not participate at the conference familiar with the focus of your research in this field?

For several years so far, I have been involved in research in the field of (e.g. acoustic) wave propagation. The mathematical models describing these phenomena were developed a relatively long time ago, and improving numerical methods and computer performance allow us to solve them better and faster. However, these problems are still hard to solve for practical applications. The same can be said for many aeroelastic or flow problems. The reduced models allow us to use differential equations and discretization methods, which have been developed over centuries and decades, as well as learn from the solution of a particular problem, a bit in the spirit of machine learning.

Has any particular research presented by the other speakers captured your attention so far?

It is difficult to name only few of them, but with respect to the topic relevant to my own research I can mention the lectures on preconditioning by Daniel Loghin and Ludmil Zikatanov, on solving the system with 200 billion unknowns by Lubomír Říha, and a slightly philosophical lecture by Zdeněk Strakoš.

Browsing your website, we have found out that you enjoy travelling and taking photographs. If you had no limitations, what places would you like to visit and photograph?

If my body did not limit me, I would climb many of the high mountains I at least hike around. My other passion is deserts, and I will certainly visit the Namib Desert, Altiplano in Bolivia, and tour the Silk Road through the Taklamakan Desert in China.

Thank you for the interview and we wish you good luck on your travels.

Jack Dongarra, nestor of HPC and the world around supercomputing visiting IT4Innovations' booth at ISC 2017

REPORT FROM THE INTERNATIONAL SUPERCOMPUTING CONFERENCE 2017 AND EVALUATION OF THE CURRENT TOP500 RANKING

Salomon is still in the top hundred. Currently in 78th place.

Participating in the International Supercomputing Conference (ISC) is slowly becoming a tradition for IT4Innovations. We had our first booth at the ISC in Leipzig in 2014 and we have participated every year since then. From 2015, the conference has been held in Frankfurt am Main. This year was the fourth time we presented our infrastructure and research to visitors at this, the biggest European event focused on HPC and its associated technology and research. This year we also participated in the presentations of the Horizon 2020 projects in which we are involved, ANTAREX and PRACE-5IP.

One of the major events that are part of the ISC every year is the announcement of TOP500's supercomputing list. China is still at the top of the list thanks to its two supercomputers, Sunway TaihuLight, with a Linpack performance of 93 petaflops and Tianhe-2 with nearly 34 petaflops. Third place belongs to Piz Daint supercomputer from the Swiss National Supercomputing Centre. Piz Daint was upgraded, doubling the Linpack performance of the system to 19.6 petaflops and enabled the system to climb five positions in the rankings.

Vít Vondrák presenting IT4Innovations at Intel's booth

Presentation of ANTAREX project (Horizon 2020)

As a result of the Piz Daint upgrade, Titan, a system with a Linpack mark of 17.6 petaflops installed at the Oak Ridge National Laboratory, drops to number four in the rankings. In the top 10 there are other supercomputers from the United States of America and Japan.

The most powerful Czech supercomputer, our Salomon, is still in the top hundred, currently in 78th place. Since Salomon was launched in summer 2015, it has fallen by 38 places. Salomon ranked 40th among the most powerful supercomputers on the TOP500 list in June 2015. The list is compiled twice a year, in June and in November. The November list is associated with Supercomputing Conference (SC), the largest supercomputer event in the world, which will be held in Denver this year. There we will also present Czech supercomputing and hope that Salomon is still in the top hundred most powerful supercomputers in the world.

TETRAMAX AND CLOUDIFACTURING,
TWO NEW INTERNATIONAL PROJECTS WE WILL JOIN

The following two new projects have been approved for funding under the EU Horizon 2020 framework programme: Technology transfer via multinational application experiments (TETRAMAX) and Cloudification of Production Engineering for Predictive Digital Manufacturing (CloudiFacturing).

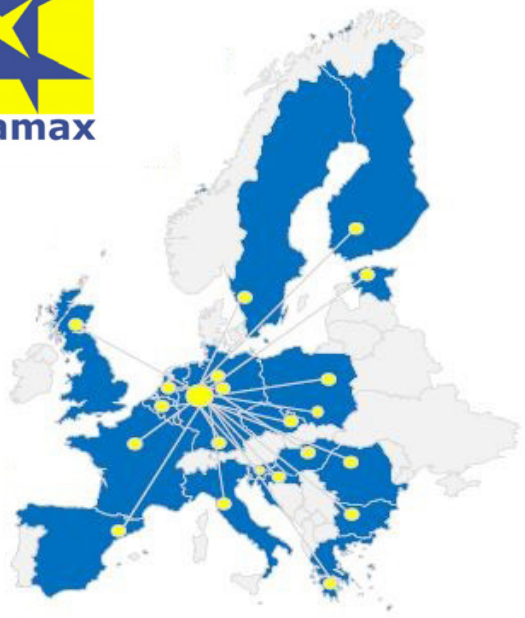
TETRAMAX

The implementation period of the Technology Transfer via Multinational Application Experiments (TETRAMAX) project will be 4 years, and its objective is to implement the European "Smart Anything Everywhere" initiative in the field of Customized Low Energy Computing (CLEC) for cyberphysical systems and the Internet of Things. The key purpose of this initiative is to accelerate innovations in European industry. The initiative connects technical and application know-how, which helps small and medium-sized enterprises adopt advanced digital technologies more effectively and efficiently.

TETRAMAX is focused on providing European industry with new innovation technologies. Therefore, the project also includes organization of several events and training sessions. In fact, the entire process of the technology transfer will be made simpler through the newly established specialized network of centres of competency in the field of very low-energy systems. The network connections will work in both directions. It will provide corporations and companies with access to advanced technologies, and research institutions will also be able to offer their technologies actively and efficiently. Within this project, the technology transfer via more than 60 international application experiments is planned.

A total of 20 research institutes and companies will collaborate in this project. The coordinator of the project is RWTH Aachen, the largest technical university in Germany. Other important European universities collaborating in the project include Delft University of Technology (the Netherlands), the University of Edinburgh (UK), Ghent University (Belgium), and the Technical University of Munich (Germany). The research centres participating in the project include the French Institute for Research in Computer Science and Automation (Institut national de recherché en informatique et en automatique, INRIA) and the Jožef Stefan Institute (Slovenia). The project partners include companies such as AMG Technology OOD (Bulgaria), Control Data Systems SRL (Romania), and Techmo sp. z o.o (Poland).

TETRAMAX consortium



In the TETRAMAX project, a key specialization of IT4Innovations is software development and multimedia data processing. IT4Innovations has at its disposal software libraries and tools, which can be useful for automotive and pharmaceutical companies, as well as for doctors in order to increase the quality of medical care.

Furthermore, we will be responsible for organizing local workshops for research partners, industrial companies, and other interested parties. Our responsibilities will also include gathering and evaluating the indicators related to dissemination and communication of the project results.

Project website: https://www.tetramax.eu/

Geographical distribution and extended coverage of digital innovation hubs, which will play a key role in increasing the efficiency of the impacts of application experiments within the CloudiFacturing project

CloudiFacturing

The objective of the Cloudification of Production Engineering for Predictive Digital Manufacturing (CloudiFacturing) project, the implementation period of which is 3.5 years, is to optimize production processes and productivity of companies using HPC-based modelling and simulation, as well as cloud services. The current trend of digitalization and the accompanying trend of production automation is also referred to as the fourth industrial revolution (Industry 4.0), in which some of the project partners are involved.

The mission of the project is to contribute to efficient use of high performance computing by European small and medium-sized production companies and thus increase their competitiveness. Small and medium-sized enterprises will have the opportunity to take advantage of the support and expertise of the researchers, and affordable access to computational resources, as the supercomputing centres have the capacity to help them optimize their productivity and production processes in the short term. The technical and economic impact of the CloudiFacturing project will be demonstrated through more than 20 international application experiments.

CloudiFacturing is a project of the European Commission initiative called ICT Innovation for Manufacturing SMEs (I4MS), which supports European leadership in manufacturing through the adoption of information and communications technologies. The new project follows the previous I4MS projects called CloudFlow and CloudSME. In the current phase, I4MS aims to extend the network of the competence centres, and their interconnection with digital innovation hubs, which will play a key role in increasing the efficiency of the impacts of the individual application experiments and the CloudiFacturing project as a whole. The digital innovation hubs participating in the project are from Hungary (Innomine Group Kft), Italy (STAM S.r.l.), Spain (Insomnia Consulting), Germany (DFKI-SmartFactory), and the Czech Republic (IT4Innovations).

In total, seventeen competence centres are defined in Europe. The four recently established centres include IT4Innovations. A total of 33 research institutes and companies will collaborate in the project. The coordinator of the project is the German Fraunhofer Society for the Advancement of Applied Research (Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V.), which is the largest European organization for applied research and development. The universities participating in the project include the University of Westminster and the University of Nottingham (UK) and Lund University (Sweden). The research organizations participating in the project include the German Research Centre for Artificial Intelligence (Deutsche Forschungszentrum für Künstliche Intelligenz GmbH), Stiftelsen Sintef (Norway), and Linz Center of Mechatronics GmbH (Austria). In addition, the project partners also include several companies, such as the Czech Ferram Strojírna company, producer of water quench machines.

The single point of access for interested parties will be an integrated digital marketplace with a clear focus on production engineering. In the digital marketplace the project partners will have the opportunity to offer their services and solutions to companies, thus making it easier for them to get access to tools developed using HPC through cloud services. The digital marketplace will interconnect people, make their collaboration easier, and provide an interactive interface for service providers.

With respect to the project needs, IT4Innovations will offer its HPC infrastructure, and contributes with its expert knowledge in the fields of modelling, simulation, and data analysis. Moreover, we will also be involved in the dissemination of project results.

IT4INNOVATIONS HAS BECOME A PRACE TRAINING CENTRE

The Partnership for Advanced Computing in Europe (PRACE) continuously aims at extending and improving educational activities and support for users of supercomputers in the field of High Performance Computing (HPC). In the PRACE-5IP project, which stands for the fifth implementation phase, PRACE has undertaken to establish and support activities of the four PRACE Training Centres (PTC) to complete the current six PRACE Advanced Training Centres (PATC), operating within important European supercomputing centres in Finland, France, Italy, Germany, Spain, and the United Kingdom. The purpose of this initiative is to complement the existing portfolio of the PRACE courses, make them geographically more accessible in other locations, and at the same time assist in developing the educational activities focused on HPC.

Seven countries, or partners representing these countries in PRACE, applied to establish a PTC. The PRACE Scientific Steering Committee has chosen the following four PTCs: GRNET in Greece, ICHEC in Ireland, SURFsara in the Netherlands, and to our intense delight, IT4Innovations in the Czech Republic, which received the best evaluation overall. The attention of the Committee was probably attracted by the substantial educational history of our centre. On average, it comprises approximately 11 courses, 14 training days, and 250 participants in each academic year, has good balance between the internal junior and renowned external lecturers, has organised several prominent international training events (e.g., PRACE summer schools), collaborates with PATC including hosting their courses, and has a convenient geographical location on the borders of the Czech Republic, Slovakia and Poland.

However, the most significant factor has been the portfolio of our own courses for PRACE, which is planned for the academic year 2017-2018 as follows:

- CFD simulations using OpenFOAM
  (9/2017, 2 days, lecturer: Tomáš Brzobohatý)
- System administration tools
  (11/2017, 2 days, lecturer: Branislav Jansík)
- Intel Xeon Phi programming
  (2/2018, 2 days, lecturer: Lubomír Říha)
- PETSc tutorial (5/2018, 2 days, lecturer: Václav Hapla)

All of these topics are relatively rare in the current PATC repertoire, which emphasizes the contribution of IT4Innovations to the PRACE educational programme. On the other hand, the advantage of our PTC status for our centre is in the potential increase in “import” of some of the top PATC tutorials, which could not be largely attended by our users otherwise.

In conclusion, let me thank all the above-mentioned and other colleagues, who are keen on sharing their extensive knowledge and expertise while providing lectures for IT4Innovations. I would also like to thank to the participants of our courses, who, despite their busy schedule, appreciate the opportunity for further professional development under the guidance of respected lecturers.

Ondřej Jakl, HPC teaching and training specialist

JAN ZAPLETAL, A RECENT PhD GRADUATE, HAS BEEN AWARDED THE JOSEPH FOURIER PRIZE FOR COMPUTATIONAL SCIENCES

Our colleague has won first place in the nationwide Joseph Fourier Prize competition for the best research within PhD studies in the field of computational sciences.

On Friday 16th June 2017, Professor Jean-Marie Lehn, Nobel Prize winner in Chemistry 1987, Roland Galharague, Ambassador of France in the Czech Republic, and Pavel Bělohrádek, Deputy Prime Minister for Science, Research and Innovation, awarded the Joseph Fourier Prize for the best PhD students in the field of computer sciences in Buquoy Palace in Prague. JAN ZAPLETAL, a recent PhD graduate from the Department of Applied Mathematics, Faculty of Electrical Engineering and Computer Science, VŠB – Technical University of Ostrava, as well as a researcher from IT4Innovations National Supercomputing Center, has won first place in the nationwide Joseph Fourier Prize competition.

At the meeting of the prize committee for the nationwide finale of the competition, which we hosted at IT4Innovations on 10th May 2017, Jan Zapletal presented his research on the Parallel boundary element method for HPC.

From the French Embassy in Prague and from ATOS IT Solutions and Services company, the winner Jan Zapletal has received a research internship in a French laboratory of his choice, and a financial award respectively. We have asked the laureate a few questions concerning the award and his studies as well as his research work at the IT4Innovations National Supercomputing Center.

What value do you attach to the received award?

I highly value the Joseph Fourier Prize for Informatics and Computational Sciences indeed. Apart from the representatives of ATOS as well as the French Embassy in Prague, the members of the Selection Committee also include experts from Czech universities. I think that the award itself is proof of the high quality of research in the field of computational sciences at VŠB. At the same time, I am happy that I have

managed to build on the achievements of my colleagues, namely Václav Hapla and Michal Merta, who, as graduates of the Department of Applied mathematics, and my current colleagues at IT4Innovations, have won the competition as well.

At the meeting of the Selection Committee, you presented research focused on the Parallel boundary element method for HPC. Can you please give the readers a simplified idea of what the boundary element method actually is?

The boundary element method is one of the methods for numerical solution of some types of partial differential equations. Similar equations serve for mathematical expression of real problems, such as sound or electromagnetic wave propagation, and heat transfer. In most cases, analytical solution of such problems is not possible, and therefore it is necessary to proceed with approximate solutions using computers. In order to do so, the boundary element is the most suitable tool to use.

What do you think was the most interesting aspect of your research, for the Selection Committee?

The application for the competition also includes a summary of my research work within my PhD studies as well as a list of publications. I think that the number of publications in respected journals was one of the main factors which influenced the Committee's decision. The crucial part of the competition, however, is the oral presentation at the Committee meeting. In this regard, I could have profited from my active participation at several international conferences and workshops, where it is necessary to present the added value of your research work to the audience in relatively short time.

What purpose does the BEM4I library, the development of which you are part, serve?

The library implements the above-mentioned boundary element method (BEM). As opposed to the frequently used finite element method, which is part of many open-source as well as commercial software products; there are not that many software packages supporting BEM. In fact, the boundary element method is more suitable for solving some types of problems, such as open-space wave propagation or shape optimization. Thus, the first motivation for developing BEM4I was to create a library designated for the research conducted at the Department of Applied Mathematics and IT4Innovations, as well as for solving real engineering problems.

What is the BEM4I development team currently working on?

One of the benefits of BEM4I is the code optimization for modern HPC architectures. It does not mean, however, that it is not suitable for personal computer computations. It is just that larger problems require hardware available only in modern supercomputing centres such as IT4Innovations. Therefore, we have been involved in code modification designed to fully exploit the state-of-the-art many-core processors supporting vector data processing. The approaches used can be tested on both the Intel Xeon Phi coprocessors available via the Salomon supercomputer, and the newer generation of these processors available at research institutions in Europe and the USA.

Have you already thought about the actual research institution in France to which you might go for the awarded internship?

Unfortunately, our team is not currently actively cooperating with any French research institution. However, one attractive option for my internship would surely be the Inria laboratory, which brings quite a significant number of research groups focused on numerical methods under one roof. I am supposed to complete the internship by the end of 2019, so fortunately there is plenty of time to make up my mind.

This will not be your first foreign study and work internship. Which internships do you value most?

At the very beginning of my PhD studies, I participated at the internship at the Graz University of Technology (TU Graz) in the research group of prof. Steinbach, who is one of the leading researchers focused on boundary element method worldwide. Although it was only a seven-month long internship, it was of great importance for completing my dissertation. Moreover, since January this year, our team, along with TU Graz, have been part of the Mobility project allowing me and my colleagues mutual visits and extension of our present cooperation.

What experience have you gained from studying and working abroad?

Apart from the already mentioned internship in Graz, I have had the opportunity to participate in several conferences focused on numerical methods and HPC within my studies, and collaboration in international projects of IT4Innovations. Many of them have contributed to the development of BEM4I, whether mathematically or computationally. To a large extent, our research has lately been influenced by the IXPUG workshops organized by the Intel Corporation. There, the participants share their early experience with HPC applications development on modern many-core processors, which has helped us prepare the BEM4I library for similar architectures.

You are currently working as a researcher in the Parallel Algorithms Research Lab. What are your future career objectives?

In the first instance, I am glad to have had the opportunity to participate in research at IT4Innovations from the beginning of my PhD studies. This allowed me and the BEM4I team to extend the library with not only the modules directly following my dissertation topic, i.e. electrical field modelling and 3D shape optimization problems, but also the modules designated for solving other problems at the Department of Applied Mathematics and IT4Innovations. However, part of my laboratory work is not only the BEM4I development – I have recently joined, for instance, the Intel Parallel Computing Center programme, dedicated to optimization of algorithms for new processor architecture, and the READEX project aimed at energy optimization of HPC applications. In the future, I would like to continue in HPC research and development, particularly solving my own projects focused on massively parallel solution of partial differential equations.

We congratulate you for the award as well as your successful completion of your PhD studies. We wish you success in your career and thank you for the interview.