IT4Innovations national supercomputing center

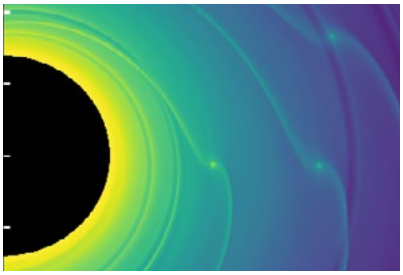
NEWSLETTER

Q2 2018

Introduction to new IT4Innovations values, mission, and vision

With respect to not only the progressive evolution of IT4Innovations but also the demands of the Czech and European research community, and gradually increasing digitalization of the whole society, we have decided to update our strategic goals, including our mission and vision, for the upcoming period 2018-2020. In harmony with the new mission and vision, we have also defined the values that we consider crucial for both our work, and successful fulfilment of our mission.

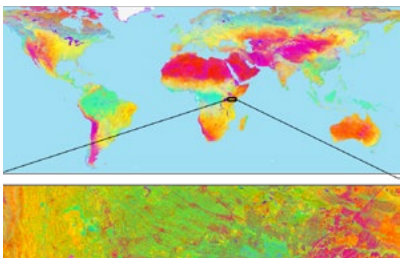
Read more



Results of the 13th Open Access Grant Competition: Who is to use our computational resources and for what

More than 55 million core hours have been distributed across 46 successful projects. We present seven of them which have won our computational resources.

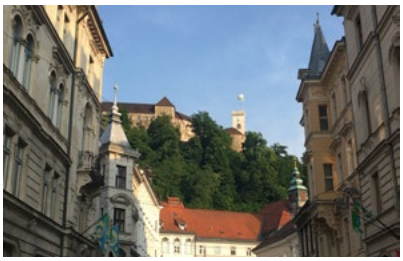
Read more



Processing and storing data for the European Space Agency

We collaborate with the German Aerospace Center, GISAT, and others within the framework of the European Space Agency project Urban Thematic Exploitation Platform.

Read more

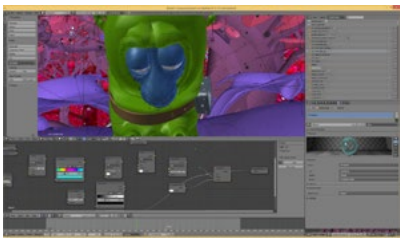


European HPC Summit Week 2018 in Ljubljana

In June we participated in the 3rd annual series of conferences known as European HPC Summit Week in Ljubljana (Slovenia), and we are pleased to bring you some details about the new things we learnt there, as well as about our contribution to the programme.

Read more

NEWSLETTER
Q1 2018



About our cooperation with the Blender Institute in development of the open-source Blender software

Our colleagues are involved in the development of Blender. It is a 3D creation suite for visualization, which covers a whole portfolio of creative functions ranging from model making and animation to final rendering.

Read more

Updated TOP500 list

It has already been the fifth time when we presented our infrastructure and research to the visitors of the largest European HPC focused event – the International Supercomputing Conference, where the latest list of the most powerful supercomputers of the world was announced.

Read more

Invitation to the 2nd IT4Innovations Users Conference

Since the launch of our first supercomputer, Anselm, in spring 2015, we have announced and evaluated a total of 26 calls for submission of applications for IT4Innovation's computational resources. More than 800 projects have been awarded computational resources. We are pleased to invite all our users to the 2nd IT4Innovations Users Conference taking place on Wednesday **7th November 2018** at IT4Innovations. Presentations or research posters, which should be registered by **31st July 2018**, are welcome.

More info

14th Open Access Grant Competition

Again, you have an opportunity to apply for our supercomputers' computational resources. The applications should be submitted by **31st July 2018**. The results of the Open Access Grant Coompetition will be announced in the second half of September 2018. The allocated computational resources will be available to the users from September 2018 to June 2019.

More info

IN BRIEF

01 Our colleagues from the Advanced Data Analysis and Simulations Laboratory participated at Transport Research Arena, the largest European conference focused on research in the transport sector, which took place in Vienna in April.

02 The Ministry of Education, Youth and Sports (MEYS), in collaboration with IT4Innovations, organized a workshop focused on the EuroHPC initiative in May 2018. For the workshop presentation, please visit the website of MEYS.

03 At the Cybernetic Revolution CZ conference, which took place in the VŠB-TUO aula on 5th June 2018, Tomáš Karásek presented the CloudiFacturing project as an opportunity for digital development of companies. For the press release accompanying the announcement of the 1st Open Call for participation in the Cloudifacturing project, please visit our website.

04 In June 2018, we represented the European research initiative Partnership for Advanced Computing in Europe (PRACE) at the biggest scientific festival in the Czech Republic, the Science Fair, which was organized by the Czech Academy of Sciences, and visited by about 24,800 people.

05 We were partners in Hackathon: Transport 4.0

06 We published a press release for the European project EXPERTISE: Advanced computational tools for turbomachinery, which provides the opportunity for 15 junior researchers to participate in 15 mutually interconnected projects.

07 The 5th anniversary of Anselm‘s launch.

08 More than 500 visitors have already been welcomed at our centre within excursions for the general public so far. Please, do not hesitate to arrange an excursion for your school/company as well by e-mail to pr@it4i.cz.

09 The 3rd annual Day of National Research Infrastructures will take place at IT4Innovations on 6th November 2018.

Dear readers,
We have recently begun comtemplating the direction in which to steer IT4Innovations in the upcoming period, what role we want to play in the Czech scientific world, and how to fulfil the mission of our national research infrastructure. Undoubtedly, we also aim to maintain and deepen our collaboration with international research organizations, and further expand cooperation with foreign institutions. We wish to build our reputation as a prestigious research institute both at home and abroad. As this process is continuous and time-consuming due to the dynamically changing R&D environment, for the upcoming period 2018-2020 we have defined new strategic goals, in the context of which we have also updated the wording of our mission and vision.

Mission
Our mission is to carry out excellent research in the fields of high performance computing and data analysis and to operate the leading national supercomputing infrastructure and enhance its efficient utilization in order to increase the competitiveness and innovativeness of Czech science and industry.
Vision
IT4Innovations aspires to be a leading supercomputing centre that provides professional services and conducts excellent research in the fields of high performance computing, and processing of advanced data sets for the benefit of science, industry, and society.

In addition, our mission and vision are supplemented with newly defined values for our institution, which we intend to recognize and honor as an institution, and which should help us achieve our strategic goals. The values are teamwork, professionalism, innovativeness, and developing a quality brand for IT4Innovations. The detailed description of these values and how they are expected to be implemented both internally and externally is described below.

Teamwork
IT4I supports teamwork; where all employees are aware that tasks and problems are solved together, and team members both respect and help each other.
Professionalism
IT4I provides professional services in all areas of its competence. All employees are accountable to their assigned work, they know their goals and actively contribute to their fulfilment, and they ensure a professional approach is maintained through regular education and development.
Innovativeness
Our employees constantly look for new opportunities for growth and development, accept new challenges, actively devise new ideas and solutions, and IT4I provides a creative environment for them.
The IT4Innovations brand
IT4I respects the standards of ethical conduct and behaviour. All employees actively participate in building and representing the IT4Innovations brand in the Czech Republic and abroad. They are proud of it, and loyal to it.

Allow me to further consider the value of innovation, which I consider vitally important for the development of our institution and society in general. I personally see it as the willingness of people to venture into unexplored areas. This naturally requires hard work, which is often at the expense of leisure time, and entails a risk of failure. In cases of success on the other hand, the resultant joy and satisfaction of creating something completely new is highly motivational. Some people may not necessarily have these ambitions, and joy when discovering or inventing something innovative does not appeal to them. However, we should have respect for anyone who embarks on this often-painful journey instead of laughing at them or trying to trip them up. Besides, I believe that success is impossible without the willingness to take potential risks. Unfortunatelly, the science funding system does not always supports this idea, and fear of the risk of failure and subsequent sanctions kills natural creativity. In the history of humanity however, far worse periods have existed. Luckily enough, we are not burned for innovative ideas so far today.

Let me wish our users as well as employees the strength of will and determination to contribute to our society with new useful inventions and applicable knowledge.

Vít Vondrák
IT4Innovations Managing Director

RESULTS OF THE 13TH OPEN ACCESS GRANT COMPETITION: WHO IS TO USE OUR COMPUTATIONAL RESOURCES AND FOR WHAT?

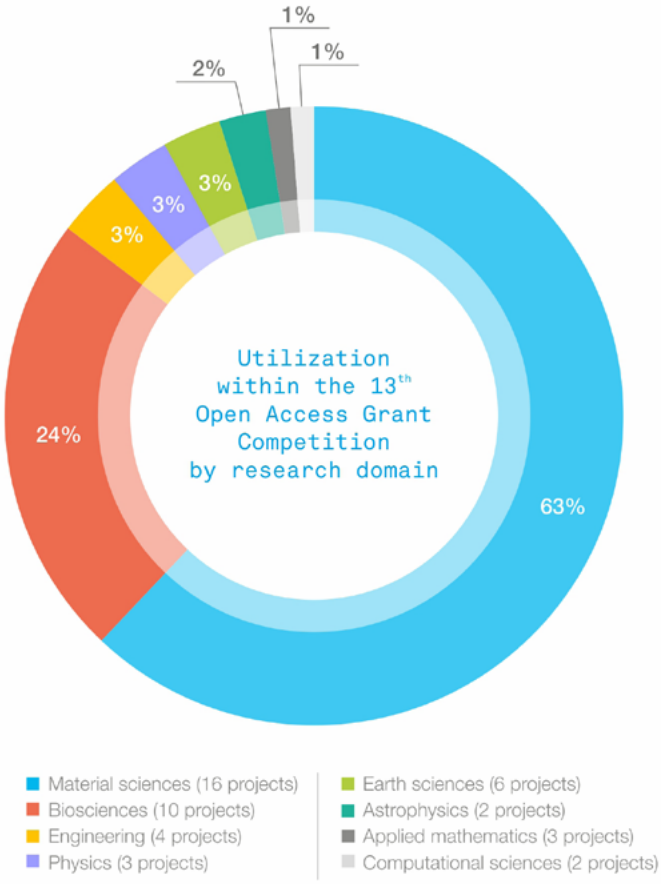
During February and March 2018, those interested in using the IT4Innovations computational resources had the opportunity to submit their application within the 13th Open Access Grant Competition. The results were announced at the end of May 2018 and successful applicants can use the awarded computational resources until February 2019. This time, more than 55 million core hours were distributed across 46 successful projects.

The largest amount of allocated computational resources was allocated to projects in the field of material sciences. Nearly 35 million corehours were distributed across 16 projects in this field. A project focused on research of the thermal expansion and conductivity of new nuclear fuels for Generation IV nuclear reactors led by our colleague Dr Dominik Legut was awarded more than 10 million core hours. The second largest allocation of 7.5 million core hours was awarded to a project focused on developing new advanced materials led by Prof. Mojmír Šob from the Central European Institute of Technology (CEITEC) Masaryk University.

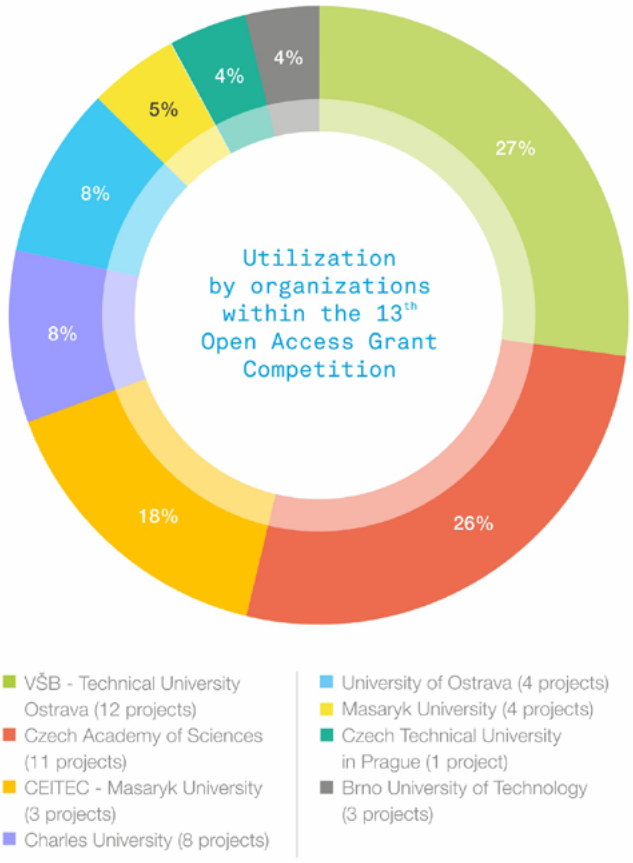
The third largest allocation of more than 3 million core hours was awarded to a project focused on reaction mechanisms of metalloenzymes, catalysts of biochemical reactions, led by Dr. Lubomír Rulíšek from the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences. His project comes under biosciences, which won the notional second place. A total of ten projects in the field of biosciences were awarded more than 13 million core hours, which makes up almost one quarter of the total allocated computational resources.

A total of 1.5 million core hours were awarded to a project focused on research of pathogenic toxins in *Clostridium difficile* and led by Dr Jaroslav Koča and Dr Petr Kulhánek, both from CEITEC Masaryk University. *Clostridium difficile* causes diarrhoea and other intestinal diseases in situations where intestinal flora is suppressed by antibiotics. The objective of this research is to aid the design of new drugs for treatment of infections caused by this bacterium.

As far as the organizations are concerned, about one quarter of the total allocated computational resources was awarded to 12 projects led by applicants from VŠB – Technical University



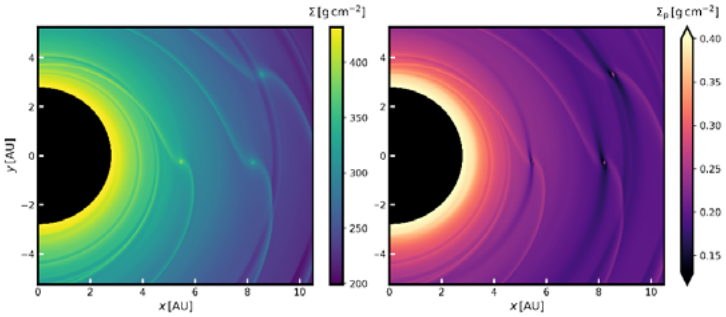
of Ostrava, including IT4Innovations. Two projects (out of 4) in the field of engineering will be implemented by female researchers from the Faculty of Civil Engineering. Ing. Zdeňka Neuwirthová will use the allocated computational resources for numerical modelling of concrete constructions interacting with subsoil. Dr Lenka Lausová will focus on numerical modelling of load of structures in quasi-static effects of wind.
The second quarter of the total allocated computational resources was awarded to 11 projects led by applicants from the Czech Academy of Sciences (CAS) institutes. They include the Institute of Organic Chemistry and Biochemistry (3 projects), J. Heyrovský Institute of Physical Chemistry (4 projects), the Institute of Physics (2 projects), and the Institute of Plasma Physics (2 projects).
Although most of the CAS projects come under materials science, the highest allocation of computational resources was awarded to three projects in the field of biosciences. Within the 13th Open Access Grant Competition, the successful projects also include those led by the applicants from CEITEC Masaryk University (3 projects), Charles University in Prague (8 projects), the University of Ostrava (4 projects), Masaryk University in Brno (4 projects), the Czech Technical University in Prague (1 project), and Brno University of Technology (3 projects).



An introduction to selected projects awarded computational resources within the 13th Open Access Grant Competition:

Dr Ondřej Chrenko (Charles University): Formation of planetary systems

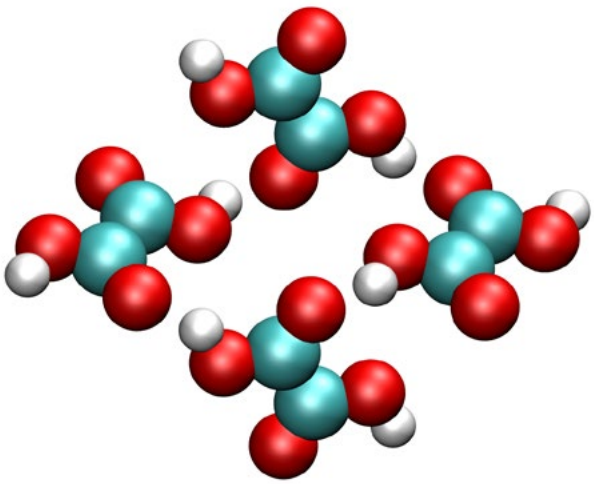
Can life be created on planets discovered outside our solar system (on exoplanets)? One of the key steps to find the answer to this question is understanding how exoplanets and their systems are formed. Possible scenarios for planetary system formation will be researched by Dr Ondřej Chrenko from Charles University in Prague. In this research project, he collaborates with other Czech astronomers Doc. Miroslav Brož and Dr David Nesvorný (working in the USA) as well as with Lund Observatory in Sweden. Using computer simulations generated by the IT4Innovations supercomputers, this project aims at researching formation of planetary embryos and their dynamic development in protoplanetary disks of dense gas and dust rotating around young newly formed stars.



Examples of RHD simulations. The colour scale in the figures shows gas surface density (left) and small solid bodies/pebbles (right). Gas and pebbles form a protoplanetary disk (only part of the disk is displayed in the figure) where planets, which rotate around the central star, are formed. In the disk, three embedded planetary embryos, which are too small to be distinguished, can be found. However, we can see the effects of gravitation interactions between the planets and the disk. It is called densification of material, and is visible in the surroundings of the planetary embryos (the three “bright spots” in the figure) where the spiral arms stem from, the disk of pebbles, and also the dark (sparse) gaps created by accretion of solid material onto the planets.

Dr Jiří Klimeš (Charles University):
Accuracy and precision for molecular solids - II

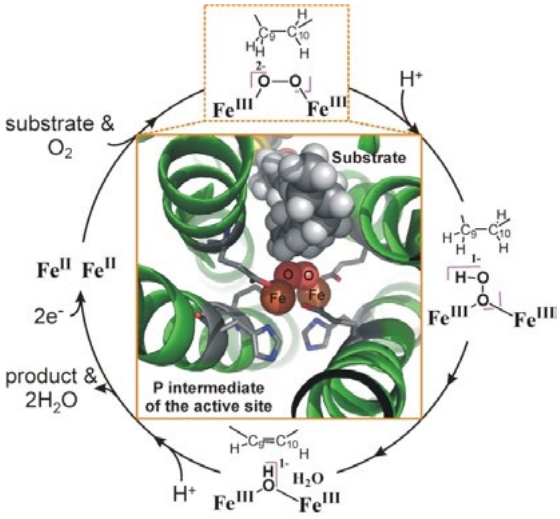
Dr Jiří Klimeš and his research team were awarded almost 2 million core hours for their development of materials simulation methods. His "Accuracy and precision for molecular solids – II project" applies quantum chemistry knowledge and approaches used for the description of solids, and received the prestigious start-up grant by European Research Council. In nature as well as industry molecular solids (molecular crystals) play an important role, for example, methane hydrate, also called Burning Ice, a potentially very important source of energy, carbon dioxide ice caps on Mars, and pharmaceuticals in pills. Some molecular crystals have peculiar yet important properties. An interesting example is polymorphism, which is the ability of a molecule of the same compound to exist in different structures under same conditions, and as such it may be crucial for effectiveness of drugs in the body.
The objective of Dr Klimeš' project is to develop methods for reliable calculations of lattice energies in materials such as molecular crystals, which will help understand their properties. In this project, the Salomon supercomputer will be used for extracting the lattice energies of 13 selected molecular crystals.



Model of the part of alpha-oxalic acid polymorph.

Dr Lubomír Rulíšek (Czech Academy of Sciences):
Reaction Mechanisms of Dinuclear Open-Shell Metalloenzymes

Metalloproteins play an important role in nature as catalysts of biochemical reactions which would not occur in the absence of metal ions. These reactions include nearly all oxidation-reduction processes, spin-forbidden processes, or processes, during which fission of very stable chemical bonds (C-H bonds, triple or double bonds in N_2 or O_2 molecules) occur. These fundamental biological processes include, for example, photosynthesis and cellular respiration.
To understand the function and structure of metalloproteins, not only experiments (e.g. x-ray crystallography, spectroscopy, and electro-chemical measurements) but also computational methods of theoretical chemistry, which can provide insights into the structure and energetic properties of metalloproteins, are important.
The project led by Dr Lubomír Rulíšek from the Czech Academy of Sciences focuses on the research of three selected metalloproteins with polynuclear cores (hence more metal ions at enzyme active sites), which play an important role not only in nature but also as potential industrial catalysts. His project was awarded over 3 million core hours. The allocated computational resources will be used for comparing experimental results with results obtained from quantum-mechanical modelling (using the Turbomole, MOLCAS, Amber, ComQum, and ORZ programs) with the objective to obtain a description of the catalytic cycles of the studied metalloenzymes. The research results have the potential to be used for biomimetic (inspired by nature) designs for catalytic cycles finding their potential area of application in the chemical industry.



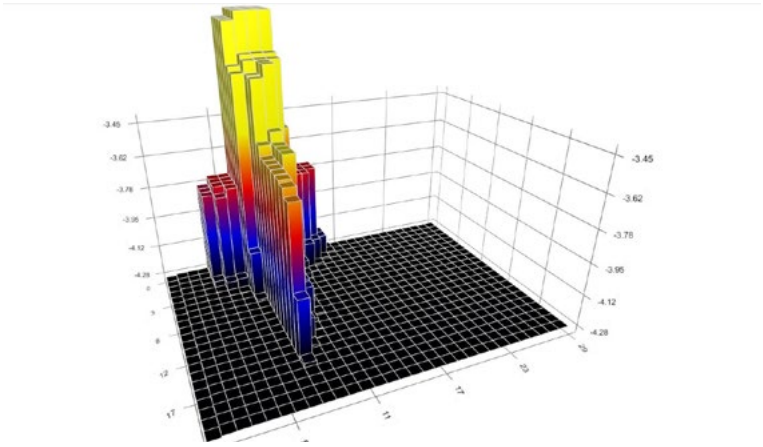
The proposed catalytic cycle of the Δ^9 desaturase

Dr Michal Podhorányi (IT4Innovations):
Parallelized reaction-transport model of contamination spread in groundwater

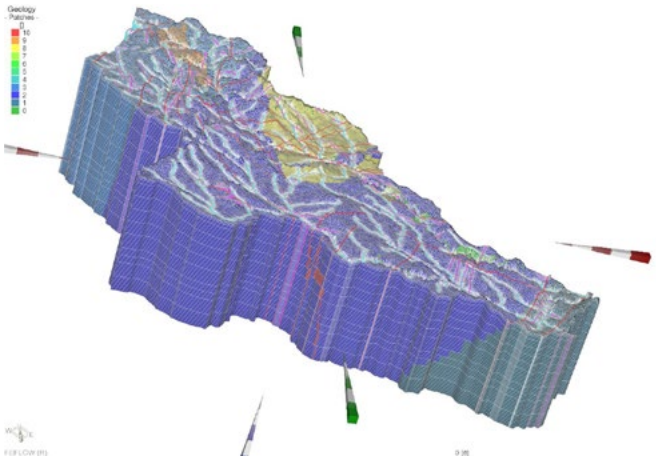
Radioactive waste (RAW) emits hazardous radiation even for tens of thousands of years. Therefore, it must be isolated from the environment for a long time until it turns into stable substances. In the Czech Republic, RAW is safely stored in three radioactive waste repositories. However, the globally most efficient and safest way for the disposal of these substances is considered to be a deep repository in a stable geological environment with the absence of natural disaster hazards, such as earthquakes and floods. In the Czech Republic, the Czech Radioactive Waste Repository Authority is responsible for the deep repository project, which is to be commenced in 2065. The Authority is currently identifying potentially suitable locations, and the final location is supposed to be selected in 2025.

Our colleagues Michal Podhorányi and Lukáš Vojáček have been cooperating with Masaryk University in Brno and the DHI company in the project titled Parallelized reaction-transport model of contamination spread in groundwater (PaReTran) supported by the Technology Agency of the Czech Republic (TH02030840). The objective of the PaReTran project is to improve methods of analyses of the potential risk of environmental contamination due to long-term spread of radioactive substances from the deep radioactive waste repository through the surrounding rock formation. Since simulations generated using reaction-transport models (FEFLOW) are computationally intensive, their parallelization for deployment on HPC systems will allow their speed-up.

The computational resources awarded in our 13th Open Access Grant Competition will be used by the researchers for the TRM program development. They will focus on testing and evaluating the scalability of the program parallelization using the open-source PhreeqcRM library for simulations of geochemical processes.



TRM model

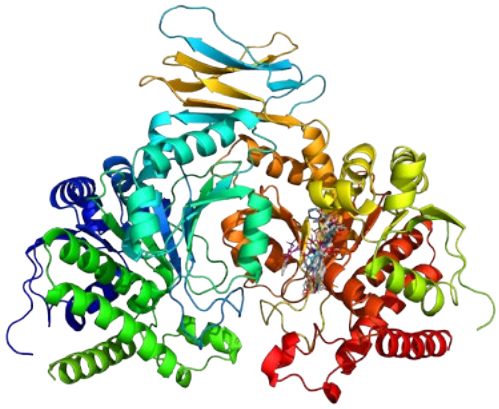


Geological model (FEFLOW)

Dr Gaspar Pinto and Jan Štourač (Masaryk University):
PredictSNP-Onco: Structural Bioinformatics Analysis for Personalized Pediatric Oncology

The research teams of Prof. Jiří Damborský and David Bednář from Masaryk University in Brno, Prof. Jaroslav Štěrba from University Hospital Brno - Children's Hospital, and Doc. Ondřej Slabý from CEITEC are involved in development of the new PredictSNP-Onco computational tool designated for personalized pediatric oncology. The new tool aims at making it faster for doctors to design the most suitable treatment for each individual patient, whose treatment so far based on standard methods has failed, or where the probability a of successful cure by standard methods is very low.
Cancer cell formation may be caused by one single mutation. Therefore, it is vitally important to assess such mutations as fast as possible, and consider treatment by all available drugs (inhibitors) which have been certified by the European Medicine Agency (EMA), the State Institute for Drug Control (SIDC), or by the U.S. Food and Drug Administration (FDA).
The computational resources of almost 800 thousand core hours will be used by the researchers to assess all possible protein mutations which lead to cancer development, and for analyses of inhibitors using the computational molecular docking method.

Using information from four world-wide databases of mutations along with the computed results, the researchers will help design new possibilities for personalized/precise treatment for various types of cancer. Doctors thus obtain information in a shorter time, which enables them to speed up the design of appropriate an treatment for each individual patient in good time.

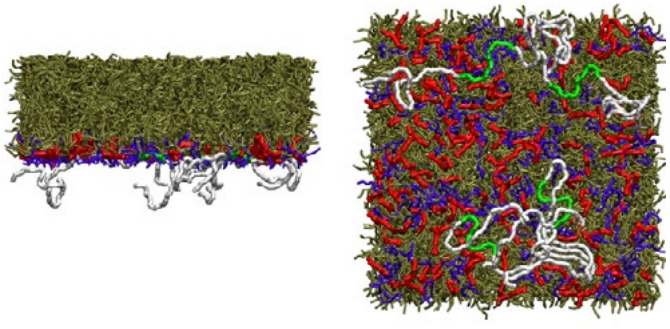


Inhibitor molecule bound in the active area of isocitrate dehydrogenase 1 enzyme (idh1)

Dr Lukasz Cwiklik (Czech Academy of Sciences):
Interactions of drug molecules with mimics of human tear film

The tear film protects the cornea of the human eye against water evaporation. It nourishes the cornea surface, and it serves as the first line of protection against eye surface infection. It is produced by spreading tears all over the eye surface by a blink of an eye. Its thickness changes during eye blinking. Essentially, it consists of a lipid and a water layer. Disorders in the lipid layer lead to dry eye syndrome, which is treated with eye drops.
The researchers from the J. Heyrovský Institute of Physical Chemistry CAS are the only ones worldwide to study the effectiveness of eye drops at the molecular level. They are seeking ways to transport the required substances through the lipid layer and cooperate with pharmaceutical companies in tear film research.
Microscopic research of the lipid layer will be supplemented with computer simulations using the Salomon supercomputer by Lukasz Cwiklik. His project was awarded more than 1.5 million core hours in our 13th Open Access Grant Competition. The allocated computational resources will be used for research of selected lipophilic drugs, in particular the way the drugs permeate through the lipid layer to the water layer.
Experimental (use of biomimetic chip, the construction of which was awarded the prestigious Neuron Impulse grant) and computational results of the research will enhance our knowledge of the interaction of drugs with the human tear film, and eventually the design of a new generation of eye drops.

For the website of Dr Cwiklik's research,
see: http://cwiklik.net



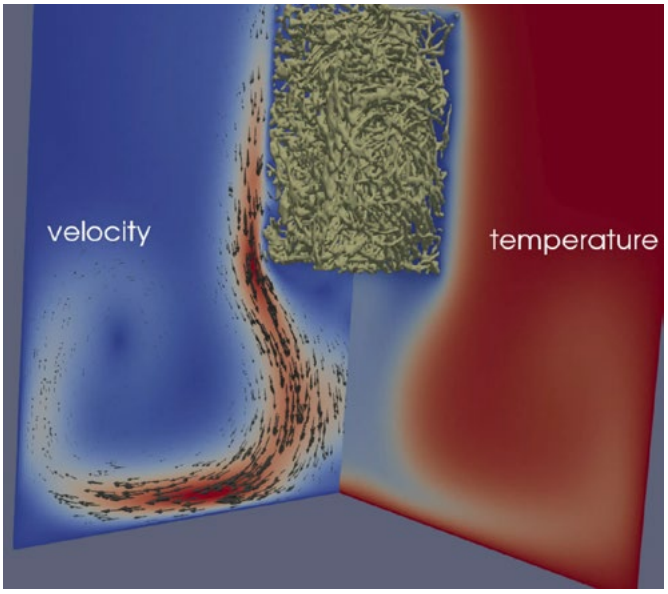
Preliminary simulations depicting the interaction
of human tear film (blue and green)
with drugs (benzalkonium chloride – in white, poloxamer-188 – in red).
Figure left: side view, figure right: bottom view.

Dr Jan Boháček (Brno University of Technology): Research centre for low-carbon energy technologies

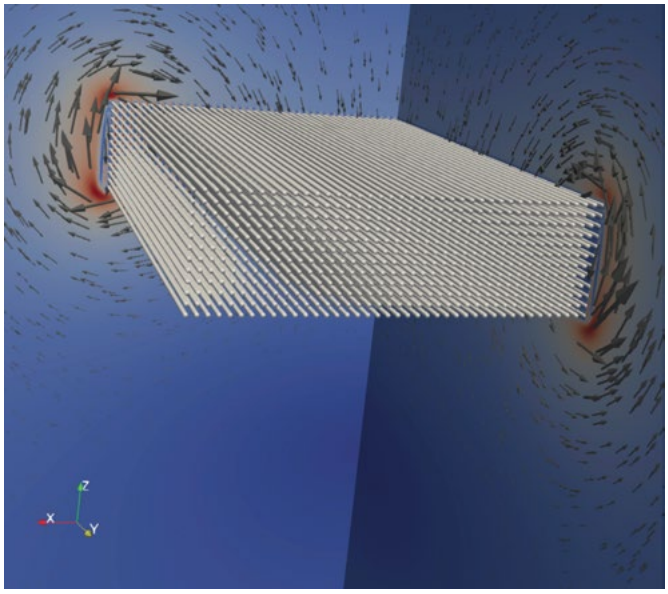
The supercomputing project of Jan Boháček from Brno University of Technology (BUT), who is involved in the five-year long project Research centre for low-carbon energy technologies (CVNET, CZ.02.1.01/0.0/0.0/16_019/0000753) supported by the Research, Development and Education Operational Programme, was awarded almost 1 million core hours.

The Heat Transfer and Fluid Flow Laboratory at BUT has been involved in the development of modern polymeric heat exchangers with hollow fibres for 10 years so far. The advantage of using polymeric hollow fibres in heat exchangers is their flexibility, low costs, and chemical resistance. Polymeric heat exchangers are ideal, for example, for heating, air-conditioning, and low-potential residual heat applications.

The allocated computational resources will be used by the group of BUT researchers for development of polymeric heat exchangers, in particular for detailed heat transfer simulations. They will analyse different factors, which affect heat transfer in polymeric hollow microfibers (diameter, lengths, and fibre spacing).

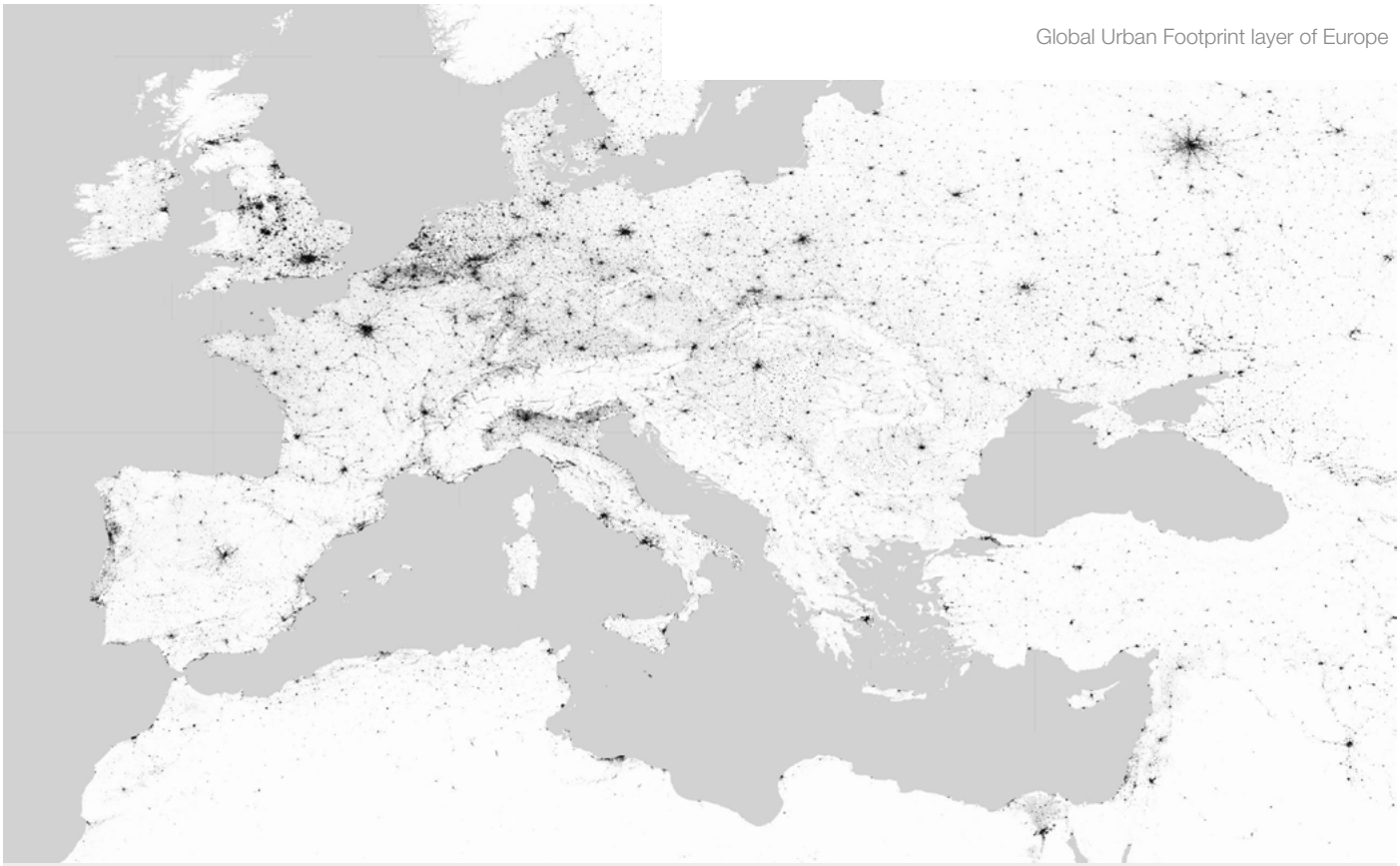


Flow around and through a porous bunch of polymeric fibres



Natural convection triggered around a polymeric hollow fibre heat exchanger

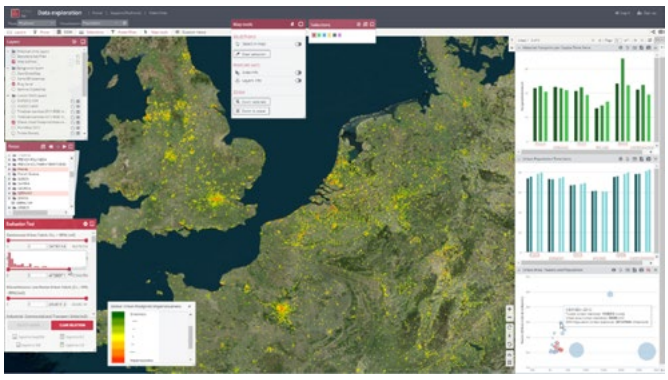
PROCESSING AND STORING DATA FOR THE EUROPEAN SPACE AGENCY



Global Urban Footprint layer of Europe

We are collaborating with the German Aerospace Center, GISAT and others within the framework of the European Space Agency project ‘Urban Thematic Exploitation Platform’.

The expanding operational capability of global monitoring from space and the challenges coming along with the sheer mass volume of data acquired by modern Earth observation (EO) missions led the European Space Agency (ESA) to launch the Thematic Exploitation Platform (TEP) initiative in 2014. In the first phase, the overall goal of the TEP programme was to develop and implement a number of thematically oriented platforms providing user communities not only with access to the mass data archives of EO missions, but also with the information and communication technology needed to effectively



U-TEP’s visualization and analytics toolbox

process, jointly analyse, and visualize them in combination with additional sources of data and information. Currently, the TEP program includes Coastal, Forestry, Geohazard, Hydrology, Polar, Food Security, and Urban platforms. IT4Innovations is involved in the Urban Thematic Exploitation Platform (Urban TEP).

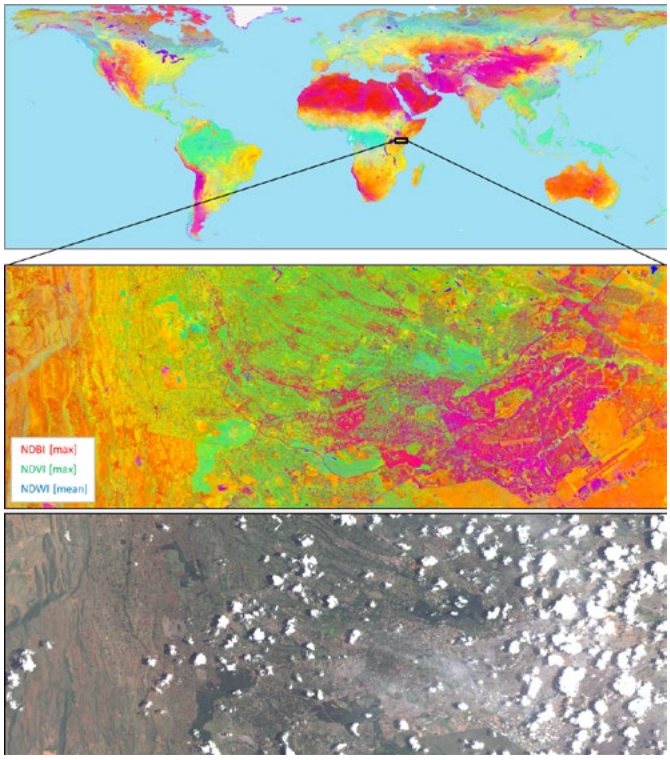
The general TEP idea follows the principle of bringing users to the data and analytics tools. Hence, the fundamental objective of the Urban TEP is to provide an open and participatory workplace where any interested (expert or non-expert) user can find end-to-end and ready-to-use solutions (data and tools) to extract unique information and indicators required for urban management and sustainability. Thematic applications includes, for example, the generation of cloud-free mosaics to provide a consistent view of the built environment, the tracing of global urbanization by means of multi-source data analytics, the quantification of regional land-use dynamics, and the deployment of processing functionalities for the derivation of orthomosaics and digital surface models from drone data.

The Urban TEP is operated by an international consortium of five partners, including the German Aerospace Center (DLR, Germany) as the lead, Brockmann Consult GmbH (BC, Germany), Terradue Srl (Italy), and IT4Innovations National Supercomputing Center and Gisat s.r.o. (Czech Republic) as partners. DLR and BC are domain experts for thematic analyses, and together with IT4Innovations, these three partners also provide the infrastructures for the data storage and data processing services. Terradue is responsible for developing the web portal and its visualization services. Gisat is developing a Visualisation and Analytics Toolbox that serves as the backbone for the joint analysis and visualization of all data layers available on the platform.

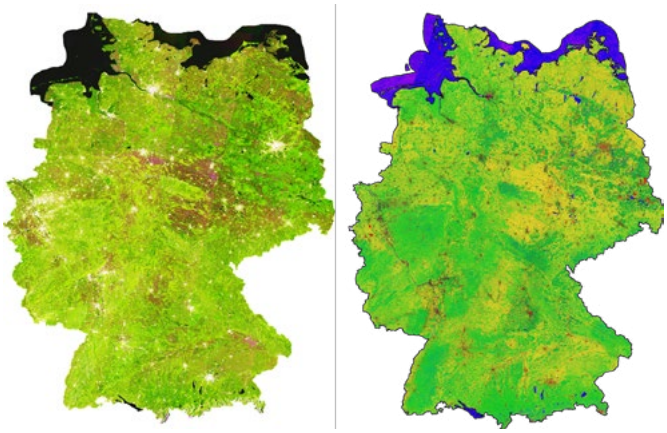
By the end of the Urban TEP pre-operations phase in June 2018, over 300 institutions from more than 40 countries will have requested products, services, and system access, with about 40 % of the users coming from the science sector, 30 % from public institutions, 20 % from non-profit/non-governmental organizations, and 10 % from the commercial sector.

In the next phase, the Urban TEP activities will focus on a systematic enhancement and streamlining of the platform capabilities and product/service functionalities to meet the requirements of a fully operational and sustainable platform.

https://urban-tep.eo.esa.int



Global TimeScan-Landsat-2015



TimeScan products for Germany derived from Sentinel-1 (left) and Sentinel-2 data (right)

EUROPEAN HPC SUMMIT WEEK 2018 IN LJUBLJANA

Between 28th May and 1st July 2018, the third annual series of conferences known as European HPC Summit week was held at the University of Ljubljana, Slovenia. The week-long summit was packed with presentations, workshops, discussions, and trends in the field of HPC in Europe. Its objective was to find synergies among all participating parties within the HPC ecosystem. Throughout the week, the summit offered workshops from several European initiatives, and presentations focused on development of various scientific fields as well as research projects funded by EU programmes. Moreover, it provided representatives of private enterprises with an opportunity to present their ideas as well.

The summit programme was initiated by the European Extreme Data and Computing Initiative (EXDCI), the objective of which is to support development and implementation of the common strategy for the European HPC ecosystem. Mark Asch from the University of Picardie Jules Verne (France), for example, informed the audience about development of activities within BDEC (Big Data and Extreme-Scale Computing), where the European Union collaborates with the United States of America and Japan. This initiative is focused on leading big data and extreme-scale computing workshops, the purpose of which is systematic mapping of how the main big data relevant issues affect national (and international) efforts to build a path towards exascale computing.

On the second day, a series of industrial and scientific presentations were carried out under the umbrella of the PRACE – PRACEdays18 project. Anwar Osseyran, the Chair of the PRACE Council and the CEO of SURFsara, the Dutch national supercomputing center, welcomed conference participants with an overview of PRACE and the statistics of its calls. PRACE currently has 25 members. The Czech Republic belongs to group of 20 main members providing

Jan Martinovič with his ExCAPE project presentation at the poster section of the conference.

support to users of Tier-0 systems, which are operated by France, Germany, Italy, Spain, and Switzerland. Since the establishment of PRACE, a total of 17 calls for project submissions have already been announced. The majority of successful projects are from the fields of materials science, chemistry, and engineering. Within the last (16th) call, almost 1.5 billion core hours were allocated to the successful applicants by PRACE. The upcoming 18th call will be launched in September 2018.

The summit participants were also welcomed by the representatives of Slovenia and the European Commission: Maja Makovec Brenčič, the Slovenian Minister of Education, Science, and Sport, Igor Papič, the University of Ljubljana Rector, and Leonardo Flores Anover, the European Commission representative who participates within DG CONNECT, which is responsible for establishing the EuroHPC joint undertaking. (Note: For more details about EuroHPC, see the previous edition of our newsletter: https://www.it4i.cz/wp-content/uploads/2018/04/Newsletter-Q1-2018-EN-preview.pdf. Another speaker at the summit was Thomas Skordas, the Director of the DG CONNECT's Digital Excellence and Science Infrastructure of the European Commission, whose presentation was titled The European HPC Strategy and the EuroHPC Joint Undertaking. Skordas mentioned that despite their efforts, the European Union does not possess the most powerful supercomputers in the world. In addition, the existing high performance computing systems are dependent on non-European component suppliers. In order to implement the EuroHPC initiative, a joint undertaking will be established. This will enable the EU to unify national and European funding together with funds of European industrial investors. The aim of this initiative is to launch an exaflop supercomputer by the end of 2023, thereby ensuring independent, competitive supplies of HPC technologies and the achievement of excellence of supercomputing applications.

Enough space was also given to presentations of experts from academia and industry, who presented advanced results from various areas of application, where use of supercomputers is crucial. To name but a few: computational fluid dynamics and engineering, materials science, and chemistry.

In the industrial section of the conference, two successful examples of the SHAPE (SME HPC Adoption Programme in Europe) programme, the objective of which is to support small and medium-sized enterprises in using high performance computing systems, were presented. In this section, an opportunity was also given to Tomáš Karásek, the Head of our Parallel Algorithms Research Laboratory, to present our cooperation with ING Corporation in creating a semi-automated workflow of modelling child cranial remodelling ortheses.

http://www.prace-ri.eu/hpc-access/shape-programme/

On Tuesday, the results achieved so far of the still running three-year ANTAREX, READEX, and ExCAPE projects supported by the European Union Horizon 2020 programme were presented. We participate in the implementation of these projects. Jan Martinovič, the Head of our Advanced Data Analysis and Simulations Laboratory, presented the ExCAPE project, within the frame of which we are involved in aiding development of scalable algorithms applicable in exascale supercomputing systems. The algorithms are developed for solving complex problems in pharmacology with respect to the necessity of processing the large amounts of data required for industrial drug development. Within the implementation of the ExCAPE project, the HyperLoom software is being developed by our colleagues for simple data processing using high performance computing systems.

The ExCAPE project website: http://excape-h2020.eu/

Promotional video explaining the project's activities: https://vimeo.com/256141454

Open source HyperLoom software: https://code.it4i.cz/ADAS/loom

On Wednesday, the European Technological Platform for HPC (ETP4HPC) we joined two years ago organized a workshop on Energy Efficiency in HPC. ETP4HPC, among others, addresses the increasingly urgent problems associated with energy consumption in exascale supercomputers. ETP4HPC members, including our colleagues, relentlessly work on developing new methods and scenarios, by means of which software as well as hardware parameters for efficient energy consumption are changed. (Note: For example, the READEX project www.readex.eu)
On Wednesday, the Memory-centric architectures (MCA) for the exascale era workshop of a private transnational company was held. The idea of MCA systems is that their own memory system will run independently on the central processing units (CPU).
Thursday's programme of the summit was initiated by Tomi Ilijaš from the private Slovenian supercomputing centre Arctur, which is the coordinator of the SESAME Net project we were also involved in. The event of the 2018 PRACE Ada Lovelace Award was held, with the winner being Xiaoxiang Zhu, a professor from the German Aerospace Center and the Technical University of Munich. She is involved, for example, in research of HPC-generated satellite images from Earth observation and their use in predicting hazards induced by degradation of constructions and damage to buildings in urban areas.
Furthermore, the 3rd Regional InnoHPC Workshop was held in Ljubljana. The objective of the InnoHPC project funded by the Interreg DANUBE transnational programme was to introduce possible uses of HPC to Slovenian companies for their innovative growth. The workshop took place at the Chamber of Commerce and Industry of Slovenia. The workshop itself was preceded by several hour-long meetings of the project partners, who discussed the project's development so far. At the Regional Workshop, the participating Slovenian companies were presented specific use cases of cooperation between companies and HPC centres. Tomáš Karásek presented our cooperation with companies in development of railroad seats and hydraulic lifts for lifting vehicles and others. Our main role in the InnoHPC project is in testing and support of the web platform allowing small and medium-sized enterprises from the eastern part of the Danube region to gain remote access to HPC infrastructures.

Project's website:
http://www.interreg-danube.eu/approved-projects/innohpc

The European HPC Summit Week not only provided a great opportunity for networking with other representatives of European supercomputing centres but also proved to be a unique means of information exchange within academia as well as between HPC users from industry.

We are looking forward to the next assembly of the conference.

ABOUT OUR COLLABORATION WITH THE BLENDER INSTITUTE IN THE DEVELOPMENT OF THE OPEN-SOURCE BLENDER SOFTWARE

Since January 2017, IT4Innovations National Supercomputing Center has been collaborating with the Blender Institute in the development of the open-source Blender software. It is a complex 3D creation suite covering the whole portfolio of creative functions ranging from model making and animation to final rendering.

Since Blender is intended to be open-source software, its source code is available. Along with that, Blender has been designed and developed from the very beginning to allow its extension through user plug-ins. These can be created in the popular programming language Python or, in cases of computationally more demanding modules, with a combination of C++ and Python.

At IT4Innovations, we started to use Blender for its numerous features during our cooperation with the University Hospital of Ostrava. The objective was to develop a tool for processing of medical data obtained by means of computed tomography (CT) and magnetic resonance imaging (MRI). This tool, which is in the form of a plug-in extension, is under continuous development, and it currently allows users to reconstruct full 3D models of selected human body tissues from input image data. The reconstructed models may then be used for further analyses, such as organ volume measurement, calculations of structural behaviour (mechanical loading of bones), and fluid dynamics (blood flow).

Within development of the medical toolset, advanced image processing algorithms have been used. Those led to utilization of parallel programming methods in order to obtain results faster. Together with that, deployment on the IT4Innovations supercomputing clusters (Salomon, Anselm) has been carried out.

Another field where Blender is used is image rendering. Rendering can create realistic images from 3D computer scences. For these purposes, Blender offers users the advanced Cycles renderer, which respects the physical laws of reflection and refraction of light. Computational intensity of even a short, realistic looking animation is enormous. Therefore, the idea of using supercomputers naturally came forward. However, Cycles was not adapted for these purposes. This fact triggered our cooperation with the Blender Institute.

In order to enable Cycles to render on a cluster, it has been extended to the CyclesPhi version, which allows the IT4Innovations infrastructure to be fully utilized, including the Intel Xeon Phi accelerators, which are embedded in approximately half of the compute nodes of the Salomon supercomputer. Cycles Phi was used within our collaboration with the Blender Institute during creation of their promotion movie Agent 327: Operation Barbershop. Salomon thus became the main supercomputing infrastructure for the final rendering of this short movie.

The movie Agent 327 was awarded the prestigious global Webby Awards in the Online Film & Video / Animation / People's Voice category (https://www.webbyawards.com/winners/2018/film-video/general/animation/agent-327-operation-barbershop/). In this context, we are also proud to mention the achievement of our colleague Milan Jaroš, the key developer of CyclesPhi, who was recognised at the 2017 International Conference on Computer Graphics and Digital Image Processing, (CGDIP 2017) for the excellent presentation of his research project titled Rendering in Blender Cycles using MPI and Intel Xeon Phi.

Milan Jaroš and his lecture on Acceleration of Blender Cycles Render Engine using Intel Xeon Phi at the Intel MIC Programming workshop, February 2017

Milan Jaroš, the key CyclesPhi developer, with the CGDIP 2017 Award

UPDATED TOP500 LIST

In June, we participated at the longest-running HPC-focused International Supercomputing Conference (ISC) in Frankfurt (Germany). Its history dates back to 1986. Previous annual editions attracted more than three thousand experts and students from all over the world. It has already been the fifth time where we have had the opportunity to present our infrastructure and research.

During the conference, the list of the most powerful supercomputers in the world was updated. Its announcement was very surprising. The new world's most powerful supercomputer is Summit, which was put into operation in the American Oak Ridge National Laboratory (in Tennessee) at the beginning of June 2018. With its theoretical peak performance of 187 PFlop/s, Summit outperforms the Czech Samolon supercomputer almost a hundred times. For the first time since November 2012, the US claims the most powerful supercomputer in the world again. Summit has shifted the Chinesse Sunway system, the theoretical performance of which is 125 PFlops, from the TOP500's leading position. Summit was funded by the Department of Energy of the United States of America, the key interest of which is research in the field of nuclear fusion, alternative sources of energy, materials science, climate computational chemistry, and cosmology. Needless to say, the world's most powerful supercomputer will also be used for medical care research (of drugs, cancer, etc.).

Summit is seven times more powerful and 5 times more energy-efficient than Titan, its predecessor. Put into operation in 2012, Titan, with its theoretical peak performance of 27 PFlops, will probably be decommisioned.

The updated list has revealed some interesting changes. A total of 133 brand new supercomputers appeared in the list. Four of the five top systems were either new or substantially upgraded.Europe claims a total of 101 computing systems in the TOP500 list, 29 of which are brand new.

The European most prominent countries are the United Kingdom, with 22 systems (total theoretical computing power of 54 Pflop/s), Germany with 21 systems, and France, with 18 systems (the total theoretical performance of systems in Germany and also in France is 64 Pflop/s).Apart from Germany, our neighbouring state Poland has its computing systems in the TOP500 list too. The theoretical performance of the four Polish systems is 6 Pflop/s.

The Czech supercomputer Salomon, which has been in operation for three years now, and is currently the only representative from the Czech Republic in the TOP500 list, is at 139th place.