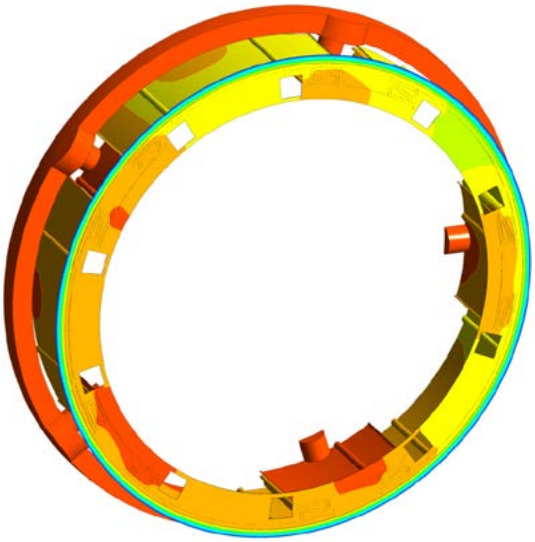
IT4Innovations national supercomputing center

NEWSLETTER

Q3 2018



About our collaboration with industry

Part of the computational resources of our centre is used within our collaboration with industrial partners from various sectors. Companies have the opportunity to both rent the computational resources of our supercomputers and use the advanced knowledge of our experts for complex solution of a specific problem. Let us take a look at the exemplary use of our supercomputing infrastructure within a collaboration with an engineering company.

Read more

Our Centre Hosts Students from All Over the World Coming to Ostrava to Participate in the Prestigious International Summer of HPC in July

This year, we proudly hosted the prestigious International HPC Summer School on Challenges in Computational Sciences, IHPCSS, with the participation of 78 students and 30 mentors from Europe, the United States of America, Canada, and Japan.

Read more

ExaQUte

Exascale Quantification of Uncertainties for Technology and Science Simulation

Computer Simulations for Future Civil Engineering

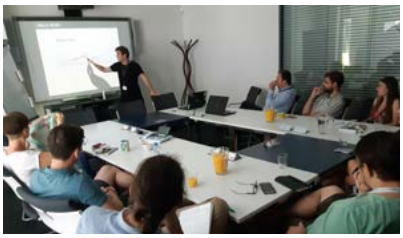
The three-year project titled EXAscale Quantification of Uncertainties for Technology and Science Simulation was approved for funding from Horizon 2020, the EU Framework programme for Research and Innovation. The objective of this project is to develop new methods for solving complex engineering problems using numerical simulations and future exascale systems.

Read more

Senators from the Parliament of the Czech Republic and Representatives of the Czech Ministry of the Interior eGovernment Department on Their Official Visit to Our Centre

The end of August was marked by an official visit of senators followed by the representatives of the Czech Ministry of Interior eGovernment department in early September.

Read more



Students From Europe Spending Their Summer With HPC

It has already been for the sixth time that students of European universities have been offered summer internships within the PRACE Summer of HPC programme. A total of 23 students were selected and participated in these internships at 11 host institutions.

Read more

INVITATIONS

Invitation to the 2nd Users‘ Conference of IT4Innovations

We remind our users of the 2nd IT4Innovations Users Conference, which will be held on **7th November 2018** at IT4Innovations National Supercomputing Center. You can register until **31th October 2018**.

More info

Call for Submission of Abstracts for the Supercomputing in Science and Engineering Publication

The users of our high performance computing systems are kindly asked to contribute to the second edition of the Supercomputing in Science and Engineering publication. The publication shall contain selected abstracts of research projects which were carried out with the support of computational resources allocated within any of our 8th through 12th Open Access Grant Competitions. The publication (with an ISBN) is scheduled to be published in the 1st quarter of 2019.

For information about the required format of the research abstracts, please see https://www.it4i.cz/call-for-abstracts-for-the-2nd-edition-of-the-publication/.
Please submit your abstracts by **30th Novembe**r to the following e-mail address pr@it4i.cz with the subject line Publication Supercomputing in Science and Engineering.

More info

The 15th Open Access Grant Competition was launched in October 2018

On 5 October 2018, the 15th Open Access Grant Competition was launched. You can apply for computational resources of our supercomputers until **30th November 2018**. The period to use computational resources obtained is expected to start on **25th January 2019** and end on **22nd October 2019**.

More info

18th PRACE Call for Project Access

The applications for Tier-O systems' computational resources within the PRACE Project Access Grant Competition shall be submitted by 3**0th October 2018**. The minimum allocation amounts to 15 million core hours. The computational resources shall be allocated for a period of one year beginning in **April 2019.**
For further information and the required forms, please see the following PRACE website.
http://www.prace-ri.eu/prace-project-access/

More info

Funding of entrepreneurial technology transfer experiments within the TETRAMAX project

The TETRAMAX project has announced its first call for funding of Entrepreneurial Technology Transfer Experiments with the aim to mobilize, challenge and train small teams of potential entrepreneurs in the Customized Low-Energy Computing (CLEC) space from a long-term perspective.. The call is open until **30th November 2018**.
For more information about the call, see the official TETRAMAX website.

More info

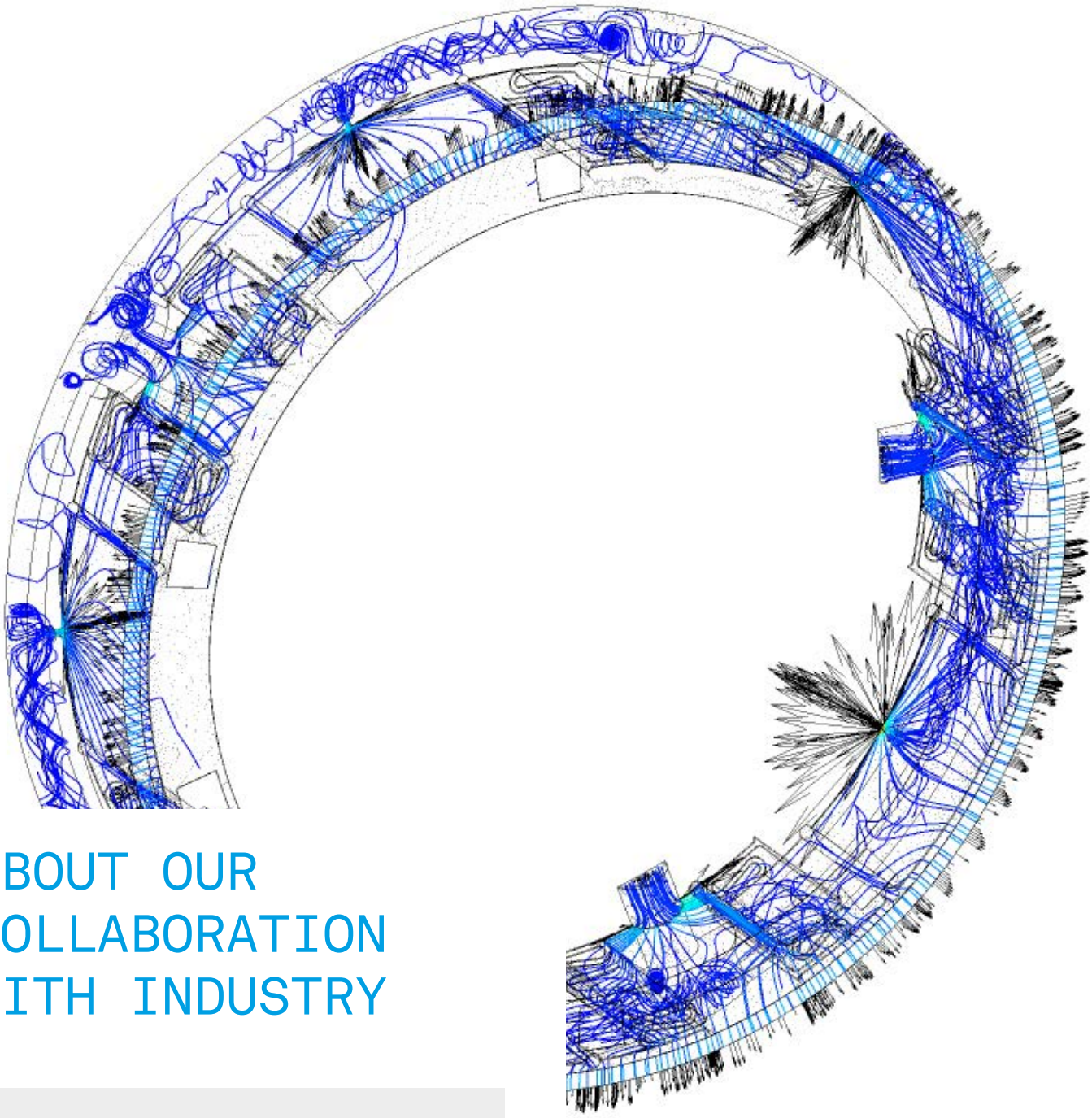
01 Czech Interview with Vít Vondrák: Europe fails to keep up in the global race of supercomputers. We want to get the Czech Republic to the top (lupa.cz)

02 IT4Innovations is registered by the European Commission as a Digital Innovation Hub for cooperation with industry in HPC and advanced data analysis. For more detailed information, see the online catalogue on the official website of the European Commission.

03 The 3rd National Research Infrastructures Day is to be held at IT4Innovations National Supercomputing Center on 6th November 2018.

04 We participated at the Art and Science festival organized by VŠB – Technical University of Ostrava on 6th September 2018. The festival aimed to uncover the beauty of science as well as the presence of science in art.

05 In the Springer database, you can find the online version of the post-conference proceedings from the international HPCSE 2017 conference organized by IT4Innovations last May. The publication contains 15 selected papers about the research projects presented at the conference.



ABOUT OUR COLLABORATION WITH INDUSTRY

A portion of of the computational resources of our centre is used during our collaboration with industrial partners from various sectors. There are several possible forms of such collaboration, selected examples of which will be presented in our newly prepared first edition of an industrial brochure.

Specific forms of possible cooperation include renting the computational resources of our supercomputers, collaborative research (co-investigators of research projects), and contracted research.

Companies can **rent** computational time on the condition that they have their own codes, and neither scientific cooperation nor assistance with their deployment and efficient running on a supercomputer are needed.

During **collaborative research**, the involved partners put their knowledge, experience, and resources into the project in order to achieve a defined goal.

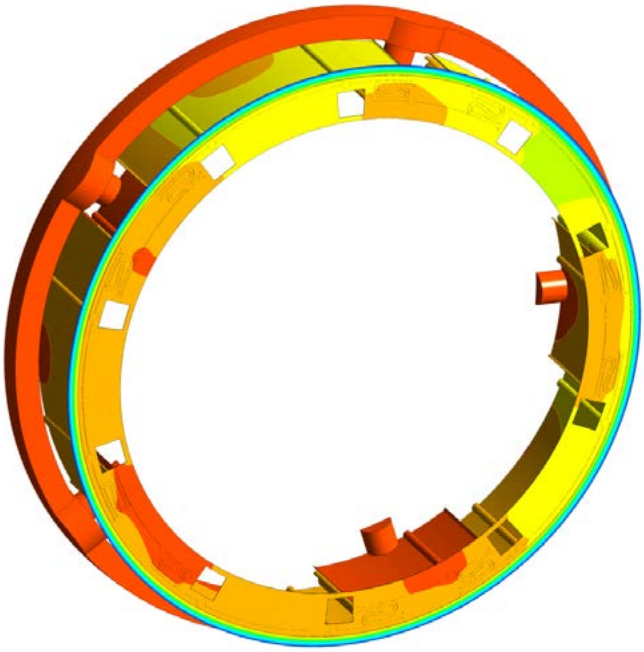
A company able to precisely define the problem they face, and which is interested in having an optimal solution developed by our colleagues, may engage in **contracted research** with us.

The companies using our services in the form of contracted research are primarily involved in the field of mechanical engineering and information technology. We also collaborate with companies operating in the health and medical technology sector, geology, geodesy as well as the environmental sector. Let us take a look at the exemplary use of our supercomputing infrastructure within the collaboration with one of the major engineering companies operating in the Czech Republic.

In collaboration with Doosan Škoda Power s.r.o. (DŠPW), we are **studying dynamical properties of the squeeze film damper**. DŠPW is a leading producer and supplier of highly efficient steam turbines with a capacity of 10 MW to 1200 MW, technological equipment, and a provider of services for the energy industry. The mutual cooperation is focused on research and development in the field of vibration damping using squeeze film dampers in rotary machines such as steam turbines.

Undesirable behaviour in the rotary machines' modes of operation, transmitted force, and maximum deflection of lateral vibration can be significantly reduced by using damping elements placed between the rotor and its stationary part. This can be achieved by using a squeeze film damper. This damping element is created by connecting the hydrodynamic and rolling element bearing, and its damping effect is generated by squeezing a thin oil film layer. There are currently several variations in the design of squeeze film dampers.

The research was focused on the state-of-the-art constructional arrangement of the damper. The main objective of the research and development process was to determine the stiffness and damping coefficients of the oil film damper. One of the efficient approaches to determine these coefficients is the use of CFD simulations. A standard workstation has proved insufficient for performing the required CFD simulations within a reasonable time limit. To illustrate this point, even when several hundreds of compute nodes were employed, it took about five days to perform a single CFD simulation. The use of the IT4I HPC infrastructure as well as the established mutual cooperation between the experts based both at Doosan Škoda Power s.r.o. and IT4Innovations in the field of CFD calculations, dynamics of rotary machines, and high-performance computing (HPC) made it possible to successfully identify the dynamic parameters of the damper. The acquired data and experience have been of great help to the industrial partner in efficient design of new constructional arrangements of squeeze film dampers.



We have asked Ing. Václav Polreich, Head of Measurements and Diagnostics, about the benefits of their collaboration with IT4Innovations National Supercomputing Center, and where would they like their collaboration with IT4Innovations to lead to in the future?

"The mutual cooperation is aimed at research and development in the field of vibration damping using squeeze film dampers, which are employed in rotary machines for attenuating undesirable amplitudes of asynchronous components frequencies, which thus contributes to more flexible and smooth running of these machines. The cooperation with IT4I researchers was very productive. They posses expert knowledge of modelling and CFD calculations. Furthermore, they have at their disposal a high-performance computing machine, which has the potential to perform CFD simulations within a reasonable time limit. Thanks to these skills and competencies, the dynamic parameters of the damper have been successfully identified.

In the future, we would like to build on this acquired knowledge in order to design a brand new radial bearing damper. The new design will be supported by CFD calculations and simulations performed by the IT4Innovations team. For verifying the computed dynamic coefficients, the test facility of Doosan Škoda Power s.r.o. will be used."

IN JULY WE WELCOMED STUDENTS FROM ALL OVER THE WORLD, WHO ARRIVED IN OSTRAVA TO PARTICIPATE IN THE PRESTIGIOUS INTERNATIONAL HPC SUMMER SCHOOL

This year, we proudly hosted the prestigious International HPC Summer School on Challenges in Computational Sciences, IHPCSS, with the participation of 78 students and 30 mentors from Europe, the United States of America, Canada, and Japan.

Students from Europe, the USA, Canada, and Japan interested in High Performance Computing (HPC) may apply to participate at the international HPC Summer School. Nevertheless, only the best students selected by the organizing institutions may participate at the summer school. The sponsors of this year's school, who cover the students' costs of travel, accommodation, and food, include American organization XSEDE, pan-European research infrastructure PRACE, Canadian consortium SciNet HPC, and Japanese organization RIKEN AICS.

The previous summer school series have taken place in Italy, the USA, Ireland, Hungary, Canada, and Slovenia. Our centre in Ostrava hosted the latest 9th summer school. It took place between 9th and 13th July with almost 80 students and 30 mentors from all over the world participating in it.

The school was officially opened on Sunday afternoon at IT4Innovations. The educational programme of the school, which was packed with lectures and practical seminars, commenced on Monday.

The seminars were led, among others, by John Urbanic from Pittsburgh Supercomputing Center in the USA, David Henty from EPCC in the UK (parallel programming), Marcelo Ponce (scientific visualizations) and Ramses van Zon (Python in HPC), both from the University of Toronto in Canada, Thomas Röhl from the University of Erlangen-Nuremberg in Germany (node-level performance optimization), and Elsa Gonsiorowski from Lawrence Livermore National Laboratory in the USA (software engineering).

Two nights were dedicated to poster sessions providing the students with an opportunity to present their research.
A total of 78 contributions from various scientific domains were heard, followed by relevant discussions.

Part of the school programme was dedicated to mentoring, with the organizers sharing their professional and personal development related experience with the students. Thus the students had an opportunity to discuss matters concerning, for example, writing final reports, improving work performance, careers in HPC, and possibilities of doctoral studies with the mentors.

For the summer school participants, two social events focused on exploration of the universe and the history of Ostrava were organized. The participants visited the Johan Palisa Observatory and Ostrava Planetarium and took a tour of the Landek Park Mining Museum.

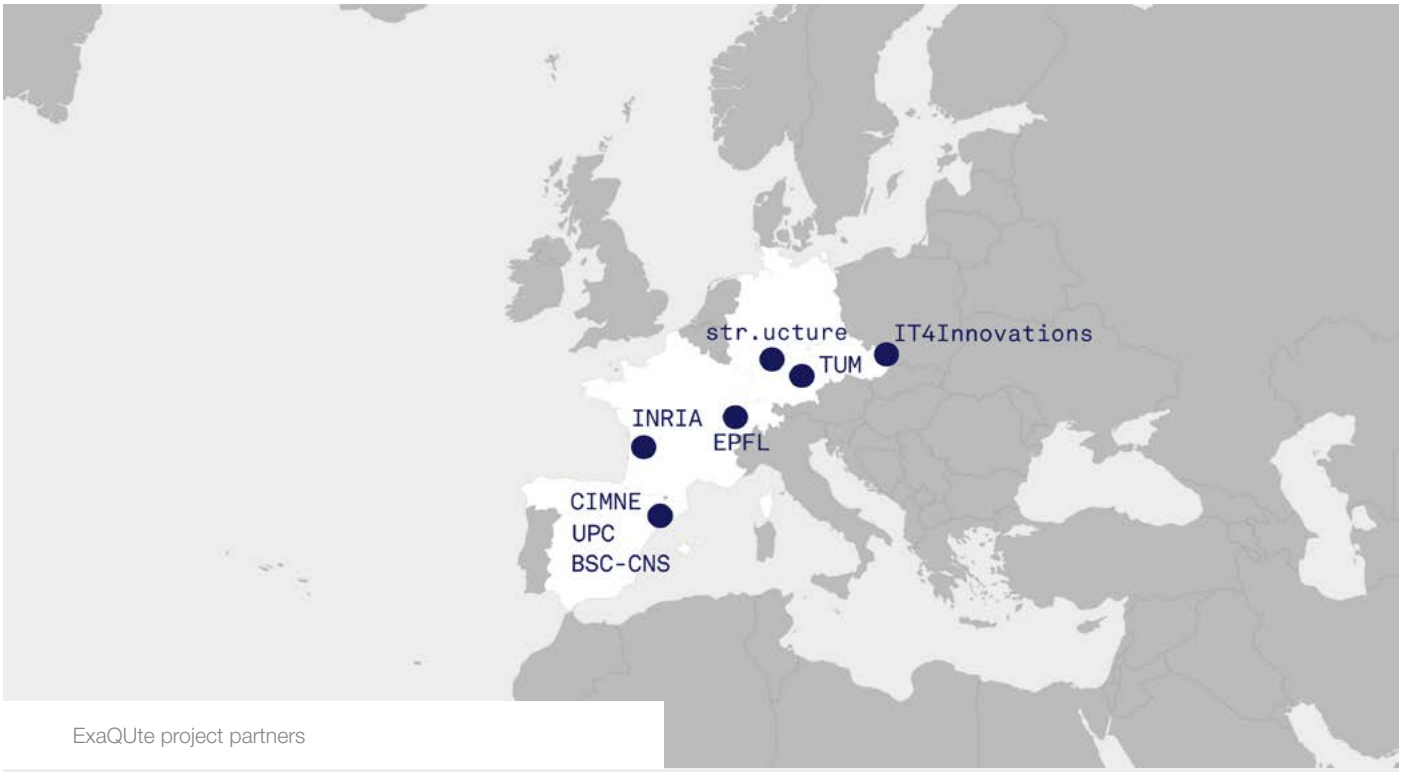
We are very pleased to have had the opportunity to host the International HPC Summer School in Ostrava this year. The entire event was sustained by a pleasant and friendly atmosphere among students and mentors. Apart from photographs, the following video capturing the course of the summer school was created:

https://www.youtube.com/watch?v=Fg4J4N4m_Vo

The Call for submission of applications for the next International HPC Summer School will open at the end of the year 2018.

http://www.ihpcss.org/

COMPUTER SIMULATIONS FOR FUTURE CIVIL ENGINEERING



ExaQUte project partners

The three-year project Exascale Quantification of Uncertainties for Technology and Science Simulation has been approved for funding from Horizon 2020, the EU Framework programme for Research and Innovation.
The objective of this project is to develop new methods for solving complex engineering problems using numerical simulations and future exascale systems. New computing methods and software tools for solving aerodynamics simulations to optimize complex geometric constructions will be developed.
Their contribution will be demonstrated on wind engineering problems.

Wind loading plays an important role in the design of engineering constructions, whether in the design of large and light constructions (e.g., stadium roofs, long bridges, narrow towers, and skyscrapers) or mechanical constructions (cranes, windmills, and electricity pylons). Large and towering buildings in cities affect the character of air flow in the system. In their design, it is crucial to correctly determine the wind load and assess its impact on the comfort of their inhabitants.

Nowadays, combinations of experimental methods based on testing in wind tunnels and stochastic analysis are used for structural shape optimization with respect to wind loading. Designers of light structures, however, face a significant **challenge**, which lies in the practical unfeasibility of experiments based on the most precise simulations of wind loading in light constructions. In order to fit such construction into a low-speed aerodynamic tunnel, it must

be significantly geometrically reduced in size. Simulation of behaviour of such size-adjusted construction models cannot reflect their real-life behaviour.

Therefore, designs of flexible and light constructions entirely depend on the personal experience of designers taking into consideration the fact that in extreme cases, **fatal failures** may occur. One such example is the Tacoma Narrows Bridge, Washington, USA, in 1940, which collapsed due to aeroelastic vibrations, another is the Montreal Olympic Stadium roof collapse in 2007 due to a heavy snowfall. Computer simulations and precision improvement of their results (not only) for light constructions thus seem necessary.

For industry, not only precision improvement of simulations but also reduction of their execution time is important. Scientists focus their research on new methods of optimization such as stochastic optimization incorporating uncertainty. As the deterministic models used so far cannot analyse random variations, stochastic modelling allowing for quantifying random variations in one or more inputs under the same initial conditions is starting to replace them.

Within the ExaQUte project, a total of eight partners from five different European countries will cooperate. Spain will be represented by the International Centre for Numerical Methods in Engineering (Centre Internacional de Metodes Numerics en Enginyeria, CIMNE) as the coordinator, Barcelona Supercomputing Center (Centro Nacional de Supercomputacion, BSC-CNS), and Universitat Politecnica de Catalunya (UPC). The German partners include the Technical University of Munich (Technische Universiät München,TUM) and mechanical engineering company str. ucture GmbH. Furthermore, the project also involves the French Institute for Research in Computer Science and Automation (Institut national de recherche en informatique et en automatique, INRIA), the Swiss Federal Institute of Technology in Lausanne (École polytechnique fédérale de Lausanne, EPFL), and IT4Innovations National Supercomputing Center to represent the Czech Republic. The project investigators from IT4Innovations are Dr Jan Martinovič and Dr Tomáš Karásek.

Within the EXAQUte project cooperation, IT4Innovations National Supercomputing Center is mainly involved in deploying the Hyperloom and COMPss tools on high-performance computing systems including their configuration and optimization. IT4Innovations will participate in testing robust algorithms for shape optimization of constructions under wind loading.

SENATORS OF THE PARLIAMENT OF THE CZECH REPUBLIC ON THEIR OFFICIAL VISIT TO OUR CENTRE

A group of 9 senators of the Parliament of the Czech Republic honoured us with a visit on Thursday 30th August 2018.

REPRESENTATIVES OF THE CZECH MINISTRY OF THE INTERIOR EGOVERNMENT DEPARTMENT WELCOMED AT IT4INNOVATIONS

In early September, the representatives of eGovernment, the Czech Ministry of the Interior department for Public Affairs Administration using modern electronic tools, visited our centre.

STUDENTS FROM EUROPE SPENDING THEIR SUMMER WITH HPC

Ten countries where the PRACE Summer of HPC participants worked this year.

Already for the sixth time, the Summer of HPC programme has offered students of European universities summer internships focused on HPC in the countries participating in the Partnership for Advanced Computing in Europe (PRACE) project. The objective of the programme is to support students in gaining experience abroad as well as with the use of high performance computing (HPC) for solving problems in their field of study. This summer, 23 students from different European universities were given an opportunity to participate in summer internships at 11 host organizations.

Before commencing their internship, students first complete a kick-off training week focused on the basics of HPC. Being held at IT4Innovations last year, this year it was hosted by the EPCC supercomputing centre in Edinburgh, Scotland. Then the students travelled to the participating host institutions, and we welcomed two of them at IT4Innovations. James Lowe, a BSc graduate of the Dublin Institute of Technology School of Electrical and Electronic Engineering, worked on the High-level visualizations of Performance Data project. The project objective was to visualize the performance data within an abstract model of communication.

Vladimir Nikolic, a student of Software engineering at the University of Belgrade, was involved in the Improving Existing Genomic Tools for HPC Infrastructure project. The project aimed at developing possible solutions for improving performance of the ABySS software, which allows a genome to be assembled from very short DNA sequences. Within the project, he also actively communicated with the original ABySS software developers from Canada's Michael Smith Genome Sciences Centre.

We asked Vladimir a few questions.

What interested you the most about the project connected with human genomes when applying for the programme?
Although I had no knowledge of bioinformatics whatsoever before applying, I was told and reading up on it seemed to confirm that there are a lot of algorithmics involved. This is indeed true, and the papers I have read on the project that I have worked on use some rather clever methods. It is interesting from an engineering perspective, in particular, because we are working with limited resources and we are trying to utilize the computing power we have to assemble the genome as effectively as possible.

How would you rate the overall outcome of participating in the Summer of HPC programme and working on the project Improving existing genomic tools for HPC infrastructure?
It proved to be a useful experience. It‘s hard to give a single rating for the whole experience, but it was positive, as you get to hang out with a fellow HPC student and work on a project of your choice. We were given a fair amount of freedom here, so we could organize our time well.

Would you recommend the PRACE Summer of HPC programme to your friends?
It depends. If they are interested in trying out HPC to see whether it‘s something they would enjoy doing, then yes. It‘s a good environment for that, as the project difficulty is adjusted to your skill level so you‘re able to explore the field. There is also blogging and filming involved, so if that‘s your thing, go for it.

Do you want to share with us your interesting career wish?
I am considering HPC as a career path, and I think scientific computing interests me the most. I‘d say that right now I‘d be most interested in working on physics simulations as it merges two fields I am interested in.

We appreciate Vladimir’s enthusiasm for his work within the project and wish him all the best in both his studies and career.

For Vladimir’s final video summarizing the results of his work within the project, see the following link.

https://youtu.be/OrendUwoEKw