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### The Results of the 9<sup>th</sup> Open Access Call

In October 2016, and in January 2017, the 9<sup>th</sup> Open Access Call and its results were announced, respectively. 49 796 000 core hours have been allocated among 41 successful projects. 84 % of all resources allocated within this call have been allocated to projects in the fields of material sciences and biosciences.

Read more



## About the conference in the northernmost inhabited place on our planet

In the first half of February, seven of our colleagues participated in the International Conference on Domain Decomposition Methods, which took place in a very interesting location.

Read more



#### Interview with Koen De Bosschere, coordinator of the HiPEAC network

We hosted the first HiPEAC workshop in the Czech Republic. The network coordinator Koen De Bosschere provided us with an interview.

Read more



#### We have joined another project supporting Small and Medium-sized Enterprises to use HPC in their development

The project is aimed at supporting Small and Medium-sized Enterprises in using HPC to accelerate innovations. The HPC infrastructure in the project includes the Salomon and Anselm clusters at IT4Innovations.

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#### HARPA project successfully concluded

The project HARPA (Harnessing Performance Variability) lasted from September 2013 to November 2016. The main contribution of IT4I to the HARPA project was to provide the HPC use case and its e-infrastructure to validate the HARPA-OS solution.

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#### HiPEAC Technology Transfer Award for our contribution to industrial practice

The awarded project was entitled Improved passive safety and comfort of passengers in railway traffic.



#### Study within the Computational Sciences MSc and PhD Study Programmes

A new feature of our Computational Computational Sciences study programmes is the opportunity to use our cooperation with Università della Svizzera italiana.

Read more

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#### INVITATIONS

#### Efficient HPC Development and Production with Allinea Tools

This workshop will demonstrate the use of Allinea tools for getting the most out of a cluster by easily identifying the biggest priorities for optimization across commonly occurring crash, memory and workload balance issues.

When: 27th April, 2017 | Venue: IT4Innovations National Supercomputing Center

Lecturer: Florent Lebeau (Allinea, United Kingdom)

More info

#### SHORTLY



02

The Ambassador of Switzerland, H.E. Mr. Markus-Alexander Antonietti, visits IT4Innovations



## THE RESULTS OF THE 9<sup>TH</sup> OPEN ACCESS CALL

In October 2016, and in January 2017, the 9<sup>th</sup> Open Access Call and its results were announced, respectively. 49 796 000 core hours have been allocated across 41 successful projects. The most computational resources, i.e. 42 016 000 core hours, have been allocated to projects in the fields of material sciences and biosciences, which is 84 % of all resources allocated within this call.

The greatest allocation of 14 000 000 core hours has been awarded to the material science project entitled Magneto--striction, magneto-elasticity and thermal expansion of Fe-Ti alloys. The second and third greatest allocations have been awarded to bioscience projects. 5 000 000 core hours have been allocated to the project of Dr. Karel Janko for research in the field of fish reproduction. The project of Dr. Jozef Hritz focusing on the research of proteins associated with neurodegenerative diseases has been awarded 3 300 000 core hours. 3 000 000 core hours have been allocated to three projects. One of them is the project of Ing. Milan Jaroš focused on reducing the rendering time and source code optimization of the Blender software, which is used for modelling and rendering 3D computer graphics and animations.



The nine Czech research, scientific, and educational institutions, which have been awarded the most computational resources of our super-computers within the 9th Open Access Call are: VŠB - Technical University of Ostrava, the Czech Academy of Sciences, Charles University in Prague, University of Ostrava, Brno University of Technology, Masaryk University, National Centre for Research, Development, and Testing in Aerospace, Tomas Bata University in Zlín, and University of Chemistry and Technology Prague.

# A selection of the projects awarded computational resources within the $9^{th}$ Open Access Call

### Karel Janko: The role of hybridization in triggering asexual reproduction in fish (5 000 000 core hours)

The researchers from the University of Ostrava will deal with a very interesting topic – asexual reproduction in fish. They will focus on the fish family Cobitidae, which are widespread throughout Europe. You may know some species of this family occurring throughout the Czech Republic: Weatherfish (Misgurnus fossilis) and Spined Loach (Cobitis taenia).

The reproductive abilities of this fish can be repeatedly disrupted by interspecies breeding. Interspecies breeding can lead to emergence of asexual fish individuals: both infertile males and fertile females, which do not reproduce sexually. In contrast, they reproduce clonally. All the asexual females need to reproduce is the presence of the sperm cell (male reproductive cell) to stimulate the egg cell development without the fertilization process. The offspring are all females, the clones of their mother.

Why are clonally reproducing individuals produced during interspecies breeding only? Does the emergence of such asexual fish individuals represent a natural evolutionary step in the formation of new species? Using the IT4Innovations supercomputers, the answers to these questions will be sought by the research team led by Dr. Karel Janko within the project entitled "The role of hybridization in triggering asexual reproduction in fish".





Cobitis taenia and cobitis elongatoides



Chromosomes of the hybrid of Cobitis taenia and cobitis elongatoides

#### Jozef Hritz: Protein-protein interactions important in neurodegenerative diseases (3 300 000 core hours)

The research team led by Dr. Jozef Hritz will use the IT4Innovations supercomputers for the research of the 14-3-3 protein complexes, which are associated with oncological and neurodegenerative diseases, such as Alzheimer's and Parkinson's disease.

On the atomic level, the static molecular structure of these proteins has already been studied using experimental techniques such as X-ray crystallography and nuclear magnetic resonance. However, their dynamics have not been thoroughly studied yet.

Study of the dynamical properties is essential for understanding the origin of these protein complexes because this knowledge allows target action to be taken in order to prevent the processes causing the development and progression of Alzheimer's and Parkinson's disease. The researchers from Masaryk University would like to describe these changes and thus contribute to the understanding of both neurodegenerative diseases.



Orbital floor fracture

## Michal Merta: BEM4I – Development of the parallel boundary element library II (350 000 core hours)

The researchers from IT4Innovations will continue to develop the library of parallel boundary element method (BEM)-based solvers. Within the previous project implementation, this (BEM4I) library was accelerated using the Intel Xeon Phi processors (Knights Corner, KNC), which complemented the already existing and operating parallelization using Open MPI. In this stage, it will be focused on further code optimization and its testing on the new generation of Intel Xeon Phi processors (Knights Landing, KNL). The objective of this project is to develop an efficient library for fast solution of boundary integral equations. The researchers will be involved in vectorization of system matrices and distributed memory parallelization. BEM4I could be used for solving real engineering problems in the field of sound propagation or shape optimization.



## Petr Strakoš: Detection and evaluation of orbital floor fractures using HPC resources (200 000 core hours)

The research team at IT4Innovations implements state-of-theart approaches to information technologies in medical diagnostic methods. They are focused on precise detection and measurement of orbital floor fractures from computer tomography (CT) scans in cooperation with the doctors from the University Hospital Ostrava. The objective of this project is to develop new, and improve existing, methods for CT scan analysis using image filtering and segmentation, and developing parallel algorithms for 3D model reconstruction. The algorithms will be applied to analysis of post-traumatic treatments of patients with eye injuries.



Signal distribution in a house calculated using the library BEM4I

For the results of the 9th Open Access Call, see <u>http://www.it4i.cz/jak-ziskat-vypocetni-cas/vysledky-9-kola-verejne-grantove-souteze/</u>

## THE CONFERENCE IN THE NORTHERNMOST INHABITED PLACE ON OUR PLANET



In the first half of February, seven of our colleagues participated in the 24<sup>th</sup> International Conference on Domain Decomposition Methods (DD). This time the conference took place in a very interesting location. The conference participants met in the little town of Longyearbyen on Spitsbergen Island, which is a part of Svalbard (formerly known by its Dutch name Spitsbergen) archipelago, sometimes called "Bear islands", located in the Arctic Ocean. The Norwegian name of Svalbard means the cold coast, and the islands are the northernmost inhabited place on our planet (78° north latitude).

In Longyearbyen, the participants of the conference had an opportunity to discuss research focused on domain decomposition methods, be it from the mathematical, computational sciences, or engineering application point of view. This year's conference was hosted by the Norwegian University of Bergen, which invited several prominent speakers such as Jed Brown from the University of Colorado, Boulder (USA), Laura Grigori from Inria Paris and Laboratoire Jacques-Luis Lions UPMC (France).

IT4Innovations' research was presented by our colleagues, namely prof. Zdeněk Dostál, prof. Tomáš Kozubek, dr. David Horák, dr. Lubomír Říha, dr. Alex Markopoulos, Ing. Václav Hapla, and Ing. Radim Sojka, giving four lectures and presenting one poster focused on development and implementation of the FETI (finite element tearing and interconnect) and TFETI (total FETI)-based domain decomposition methods. In view of the fact that the conference took place in such an exotic, arctic place, we have asked our colleague Ing. Radim Sojka about his overall impressions: "Although the conference took place far beyond the Arctic Circle, at 78° north latitude, about 1300 km south of the North Pole, the temperature did not drop below 0°C due to deep low pressure in the Atlantic Ocean. For the entire duration of the conference, there was polar night and thus we were at least glad for the semidarkness, which always occurred for a few hours around noon."

The 25<sup>th</sup> DD conference will take place in the town of St. John's in the Newfoundland province in Canada. Further information will be gradually added on the conference website http://www.ddm.org/.



Longyearbyen, Svalbard



### INTERVIEW WITH KOEN DE BOSSCHERE, COORDINATOR OF THE HIPEAC NETWORK

In March, representatives of five Czech technical universities and two companies met at the historic first HiPEAC workshop in the Czech Republic. Koen De Bosschere and Rainer Leupers, representatives of the HiPEAC network, invited to host the workshop IT4Innovations, as an organisation which co-organized the 11<sup>th</sup> HiPEAC conference (Prague, 2016) and whose employees are the most active ones in the HiPEAC network in the Czech Republic. The international HiPEAC network brings together experts in high-performance computing and embedded systems. HiPEAC has been organizing such workshops in the new EU member states since 2012.

The workshop at IT4Innovations hosted representatives of VSB – Technical University of Ostrava, Brno University of Technology, the Technical University of Liberec, the Czech Technical University in Prague, and the University of Hradec Králové. In addition, the workshop also hosted two companies, Daiteq and CODASIP. In order to make you, our readers, familiar with the HiPEAC network and its activities, we have asked Koen De Bosschere, the network coordinator, a few questions.

Koen De Bosschere is a professor at Ghent University in Belgium. His research interests include: computer architecture, system software, code optimization and software protection. His main service roles at the university include chairing the Educational Board for Computer Engineering and coordinating the student-entrepreneurship program. Prof. De Bosschere is editor-in-chief of the Association of Computing Machinery's journal on Architecture and Code Optimization (TACO). Since 2008 he has been coordinating the HiPEAC network funded by the FP7 and H2020 programmes.

### What do you think is the most valuable benefit for members of HiPEAC? Why should someone become a member?

HiPEAC is a network of 1700 experts in computing systems in Europe. Through the network, they can share ideas, disseminate their research accomplishments, make collaboration plans, and contribute to strategic vision documents for the European Commission. Students benefit from the training opportunities and from the mobility resources for junior researchers. Companies can benefit from the expertise that is available in the network, and from the recruitment opportunities the network offers. Hence, every computing systems expert can benefit from HiPEAC membership. HiPEAC membership is free. There is no excuse not to apply for it.

# You have chosen the Czech Republic for one of the HiPEAC workshops. What was the reason and are you happy with the outcomes?

Since 2012, we systematically visit the HiPEAC members in the new member states. The goal is twofold: we want to show our colleagues from the new member states which benefits HiPEAC can offer them, and at the same time, we hope to attract more members from this part of Europe. We strongly believe that many researchers in computing systems in the Czech Republic can benefit from HiPEAC membership. We are very pleased with the outcome of the meeting at IT4Innovations. Attendance was very good, and the presentations and discussions were very interesting.

# During the workshop you had a chance to listen to the presentations of researchers from 5 different technical universities and some companies from the Czech Republic. How does the Czech research in the field of high– –performance and embedded computing systems compare with the research of the colleagues from the original EU member states?

Had the presentations been anonymous, it would have been very difficult to tell whether they came from the Czech Republic, or from one of the 'Old member states'. The presentations were of excellent quality. Several research outcomes were the result of European research projects, which shows that the colleagues from the Czech Republic do successfully compete for international research funding. HiPEAC membership can further expand their network, and get them involved in even more project proposals.

#### One of your interests is student entrepreneurship. During your talk at the workshop you mentioned that students all around Europe are not very eager to start a business as their career path these days. When you are trying to motivate them to do so, what do you usually tell them?

The traditional production industry employing thousands of people is gradually being replaced by smaller innovative companies. The majority of these companies are digitised and collaborate intensively. In order to be successful in this new networked economy, universities should output more graduates with competencies that will help them to thrive in this new economy. Those are for example e-skills, entrepreneurship, innovation and others. This is a different profile to the standardized engineering and management profiles that are needed to run large companies. At Ghent University we work towards developing entrepreneurial and innovative competencies in all our graduates in a structured way. Some have already started small businesses while still studying, and we support them with free business coaching. In the computer engineering programme, our graduates created 400 jobs since 2008, which is on average one job per graduate. It turns out to be rather easy to stimulate students to consider entrepreneurship as a valid career option. It works at Ghent University. There is no reason why it should not work in Ostrava.

#### Thank you for the interview.







## WE HAVE JOINED ANOTHER PROJECT SUPPORTING SMALL AND MEDIUM-SIZED ENTERPRISES TO USE HPC IN THEIR DEVELOPMENT

The project InnoHPC – High-performance Computing for Effective Innovation in the Danube Region will focus on Small and Medium-sized Enterprises (SMEs). It is aimed at supporting them in using HPC to accelerate innovations.

InnoHPC will enable enterprises as well as academic and purely research institutions to develop cooperation in the field of supercomputing on the transnational level. The target group is Small and Medium-sized Enterprises (SMEs) in the eastern part of the Danube region. In this part of the region, in particular, the companies have limited access to HPC infrastructures, which affects the acceleration of development and implementation of innovations into practice. Within the frame of this project, a transnational platform allowing the use of HPC infrastructure will be developed, resulting in an increase in competitiveness of SMEs.

The InnoHPC project was launched on 1<sup>st</sup> January, 2017, and will terminate in June, 2019. The project activities will be divided into four stages. In the first stage, the project partners will evaluate the current level of exploitation of the regional HPC infrastructures. In the second stage, they will design and establish a transnational InnoHPC laboratory associating the regional HPC infrastructures. In the third stage, a pilot use of the InnoHPC laboratory and web platform will be realized by several small and medium-sized enterprises from the electrotechnical and automotive industry.

The leading project partner is the Faculty of Information Studies in Novo mesto (Slovenia), where the cluster Rudolf is located. This cluster has a computational performance of 13 Tflops and will be used for developing and testing the outputs of the project. Other partners of the InnoHPC project include educational and research institutions, such as the University of Rijeka (Croatia), the Technical University of Košice (Slovakia), the West University of Timisoara (Romania), the University of Ljubljana (Slovenia), and the Research Centre for Regional and Global Development (Bulgaria). The Budapest Chamber of Commerce and Industry, and the Electronic and Electrical Engineering Association of the Chamber of Commerce and Industry of Slovenia, are among the involved partners as well. In addition, the Austrian RISC Software GmbH company providing IT services to industrial companies is also involved. One of the affiliated partners is the Edinburgh Parallel Computing Centre (EPCC), which will assist the other project partners in providing training programmes aimed at closing the gap between academia and industry.

The HPC infrastructure that the project will use is represented by the Salomon and Anselm clusters at IT4Innovations. Our colleagues will also participate in developing, testing, and supporting the web platform, the use of which will provide SMEs with remote access to the HPC infrastructure. InnoHPC, in return, will enable establishment of cooperation with the companies in the Danube region.

## PROJECT HARPA: HARNESSING PERFORMANCE VARIABILITY SUCCESSFULLY CONCLUDED



The project HARPA lasted from September 2013 to November 2016. The goal of HARPA was to support next-generation embedded and high-performance heterogeneous many-core processors to cost--effectively confront variations by providing Dependable-Performance: correct functionality and timing guarantees throughout the expected lifetime of a platform under thermal, power, and energy constraints.

The project was led by Politecnico di Milano (POLIMI, Italy). Partners in the project were the Institute of Communications and Computer Systems (ICCS, Greece), the University of Cyprus (UCY, Cyprus), Interuniversity MicroElectronics Center (IMEC, Belgium), Thales Communication Group (TCS, France), Henesis/Camlin (HEN, Italy).

Some of the HARPA members during the final review in IMEC, Belgium.

In the project HARPA the HPC infrastructure of IT4Innovations was used. We supported the project mainly by the HPC use case - Floreon+ system, which was funded from the budget of Moravian-Silesian Region. Users can benefit from new technologies developed for the Floreon+ system within the project HARPA. In particular the software upgrade HARPA-OS which offers better availability and cost-effectiveness of the computations, and a higher error resilience of the system.

The basic idea is to use different levels of service management according to the situation. E.g. periods without precipitation are not computationally demanding, while in periods with extreme rain, with the danger of flooding, the computation requirements grow significantly to deliver accurate results.

The primary outcomes of the project in rough numbers are: In total, 16 journal papers with impact factor, 48 conference papers, 12 workshop papers, three patents and a book. As part of our dissemination strategy, the consortium organised 17 conferences and workshops. After the finalisation of the project, the partners planned more than ten new publications. More information is available at http://www.harpa-project.eu/



## WE HAVE RECEIVED AN INTERNATIONAL AWARD FOR OUR CONTRIBUTION TO INDUSTRIAL PRACTICE

HiPEAC annually grants the Technology Transfer Awards for research results that are transferred into industrial practice. We too, are amongst the recipients of the 2016 HiPEAC Technology Transfer Awards.

The awarded project entitled Improved passive safety and comfort of passengers in railway traffic was implemented by the research team consisting of prof. Petr Horyl, dr. Tomáš Karásek, dr. Petr Ferfecki, and Ing. Pavel Maršálek in cooperation with the BORCAD company, which offers a range of products for passenger train interiors. The objective was to develop safer seats for railway vehicles.

The scope of work within the project included the design of a new testing machine along with a software package, which allows very precise verification of the actual construction and development designs. The cooperation with BORCAD led to the design of a particular feature for existing passenger train double seats in order to comply with specific standards required in some EU countries. The subsequent computer simulations verified that the improved design complies with the safety criteria of the standard for each individual part of the human body.

In cooperation with the BORCAD company, we have jointly developed know-how in the area of numerical modelling and simulations of crash tests. We are planning to continue to cooperate in developing safer passenger train seats.

On the 2<sup>nd</sup> of March, we presented the study programme, Computational Sciences, at the University Study Programmes' Open Day

Erasmus student Joana Silva 🥆

## STUDY WITHIN THE COMPUTATIONAL SCIENCES MSc AND PhD STUDY PROGRAMMES

For the second time, students of BSc study programmes have an opportunity to apply for study within our Computational Sciences MSc Study Programme, which started in the academic year 2016/2017. A unique feature of the Computational Sciences MSc Study Programme is that students have an opportunity to use one of today's most powerful supercomputers throughout their studies, as well as during completion of their master's thesis. At the same time, students can focus on those areas which correspond to their interests and talent. Within their field of study, they have the option to choose both the subjects and the topic of their master's thesis from the four following specializations: data analysis and visualization, numerical parallel algorithms, computational physics and chemistry, and industrial applications. Throughout their studies, the students are involved in Student Grant Competition projects as well national and international projects. They not only obtain financial support but also have an opportunity to participate in valuable research. As far as the candidates for PhD studies are concerned, we offer them study opportunities within our Computational Sciences PhD Study Programme.

A new feature of the Computational Sciences study programmes is the opportunity to use our cooperation with

Università della Svizzera italiana (USI Lugano, Switzerland). Thanks to a student exchange programme, our students can spend up to one semester at their prestigious Institute of Computational Science broadening their knowledge and acquiring new skills.

The students can also use the opportunity to go studying abroad within the Erasmus+ programme. At the beginning of February, we welcomed our first Erasmus student at IT4Innovations. Her name is Joana Silva and she comes from Portugal where she studies biomedical engineering at Universidade do Porto. During the next few months, Joana will be cooperating with our colleagues from the Parallel Algorithm Research Lab, developing advanced tools based on the needs of doctors and surgeons with the aim of improving the quality of medical care.

The applications form for the MSc and PhD study programmes should be submitted by 30<sup>th</sup> April, 2017 and 30<sup>th</sup> June, 2017, respectively.

For the website of the Computational Sciences study programmes and guidelines for the application form submission, see http://studium.it4i.cz.