IT4Innovations
Centre of Excellence

HOT NEWS

ITS NAME IS ANSELM

The IT4Innovations National Supercomputing Centre’s first supercomputer was named after Ostrava’s first mine. The naming ceremony took place on 24 May. The name was selected from more than 6000 entries that had been submitted to the competition by the general public.

The choice resonated mainly with Ostrava’s patriots. Rector Ivo Vondrák, a member of the committee, explains the name selection on his blog. “The first mine and the first supercomputer. How do we establish a connection? It is simple – through the name Anselm.”

Anselm has already begun to serve its mission. In late spring, we allocated a total of 7,340,500 core hours within our Access Competitions, both Internal and Open. Successful applicants have already been granted access, so Anselm finally has the opportunity to show what it can do.

Ladies and Gentlemen, Dear Colleagues,

Our first machine is called Anselm. The name is meant to connect both the historical and the new that our supercomputer stands for. Anselm was the name of Ostrava’s first adit mine in which a steam engine was used for the first time in the region. By the way, at that time, chimneys and rising smoke were a symbol of prosperity. I believe that the supercomputer will mean the same thing to us that coal meant to historical Ostrava – a new period of prosperity and success. And just as new mines used to be opened and named, we will give the same names to our new high performance clusters. This is our way of paying a well-deserved tribute to Ostrava, the city of winding towers and – most recently – also a supercomputer.

Anselm is already hard at work. It is being used for supercomputing by newly built centres of excellence in research – Prague’s ELI and Brno’s CEITEC, and institutes within both the Academy of Sciences and the Czech Republic’s largest universities. We are also collaborating on research and development projects with commercial companies. For example, one of our most recent partners is Intel. It was our collaboration with Intel and other institutions that helped us succeed in prestigious calls within the Seventh Framework Programme of the European Union, allowing us to be the Czech Republic’s only successful applicant in High Performance Computing.

I wish you a pleasant day,

prof. Ing. Ivo Vondrák, CSc.
Rector of VŠB – TU Ostrava

Award-winning participants of the “Find a name for supercomputer” competition
And what do our supporters make of the name?

One for all, a post from our Facebook page:

Petr Kotas

Just as many generations of our great-grandfathers, grandfathers and fathers used to go down the mines in search of ‘black gold,’ our contemporaries will mine for valuable knowledge on Ostrava’s new supercomputer. The new machine was officially named last Friday. And since Ostrava is a distinctive region, the naming ceremony was also distinctive and short. The atmosphere was underscored by cool, drizzling rain and a crowd anxiously awaiting the new name – a name that will become a symbol of supercomputing in Ostrava for the next two years. And indeed, once the unavoidable “official theatricals” were done and over with, the first rows learned the chosen name; a name that will certainly raise a lot of conflicting questions and feelings. After a moment of silence disturbed only by the furious clicking of camera shutters, most already understood what those selecting the name had understood. It is short, it is distinctive and it is as hard to get out of your head as a pickaxe. In short, the name Anselm belongs here.

www.facebook.com/it4innovations

The supercomputer’s godparents publicly announce its name. From the left: Managing Director of IT4Innovations Martin Palkovič, Chairman of the IT4Innovations’ Managing Board Evžen Tošenovský, Mayor of Ostrava Petr Kajnar, President of the Moravian-Silesian Region Miroslav Novák, The Minister of Education, Youth and Sports Petr Fiala, and speaking at the microphone, Rector of VŠB – Technical University of Ostrava Ivo Vondrák

Nearly 150 guests accepted an invitation to Anselm’s naming ceremony

Cutting the supercomputer
Introduction to supercomputing

About forty attendees of the Introducing the Supercomputer afternoon lecture used the opportunity to learn more about supercomputers.

They peeked into the history of supercomputing and got to know Anselm, the first supercomputer operated by IT4Innovations. The lecture was followed by a lively discussion focusing mainly on supercomputing applications in various scientific disciplines. The participants were also interested in the practicalities of the supercomputer’s everyday operation.

The highlight of the afternoon was the opportunity to closely examine one blade server – a compute node, which is the basic building block of a supercomputer. One such node at our facility delivers a performance of approximately 1.096 TFLOP/s (NVIDIA accelerator version) or 1.086 TFLOP/s (Intel Phi accelerator version).
IT4I succeeds in the 7th Framework Programme as the Czech Republic’s only successful applicant in High Performance Computing

IT4Innovations research teams notched two successes in the most recent calls of the Seventh Framework Programme of the European Union, and will soon become involved in new projects. In High Performance Computing, our success was underscored by the fact that we were the only institution from the Czech Republic to receive support.

EXA2CT
(EXascale Algorithms and Advanced Computational Techniques)

The project aims to address the challenges posed by the rapid advancements in supercomputing. The next generation of supercomputers, i.e. exascale machines will require new approaches to software programming and development. The EXA2CT project brings together leading experts in the development of solvers and related algorithms, and HPC software architects, who will be programming new models and communication for new-generation supercomputers. Ten companies including Intel will participate in the project.

- Project leader: IMEC, Belgium
- Project start: September 2013
- Duration: 36 months
- Output: Innovative approaches to solvers and model programming for ‘exascale’ supercomputers

HARPA
(Harnessing Performance Variability)

The aim of the project is to design and develop methods for effectively solving problems relating to load distribution on heterogeneous multi-core systems in order to ensure the proper functioning and availability of these systems. The result will be a technical layer that will measure and identify the system's performance, power consumption, thermal constraints, durability and structure, and – based on these data – optimize the system's operation while respecting the constraints specified. A major benefit of the HARPA project lies in combining the methods that are used in embedded and HPC system domains into a single solution. The HARPA project will also demonstrate the benefits of combining the techniques of these two domains on key applications, including the FLOREON+ system that is being developed at IT4Innovations.

- Project leader: Politecnica di Milano, Italy
- Project start: September 2013
- Duration: 36 months
- Output: A technical layer that provides optimum load distribution on heterogeneous multi-core systems with respect to system performance, availability, power consumption, durability and structure
Chemists receive the largest portion of Anselm’s computational resources in the Open Access Competition

In April, 4,965,500 core hours were allocated within the 1st Public Access Call. The largest portion (3,474,500 core hours) was allocated for computational chemistry projects. In addition, physicists and mathematicians were among those who seized the opportunity to use the computational resources of the supercomputing centre in Ostrava.

The largest allocation of 2,000,000 core hours was awarded to professor Koča of CEITEC for research in enzymes. The second largest allocation was awarded within the field of physics. At the Institute of Physics of the Academy of Sciences of the Czech Republic, a team led by Dr. Ondřej Klimo will use the allocation for simulating particle acceleration by laser pulses.

The next Public Access Call is scheduled for the autumn of 2013 and it will be open to employees of Czech scientific and research institutions. All applications are subject to scientific, technical and economic assessment and, based on the results, computational resources will be allocated to successful applicants.
Examples of projects that were allocated computational resources within the 1st Open Access Competition:

**ENZYMATIC REACTION MECHANISMS INVESTIGATED BY CAR-PARRINELLO AB INITIO DYNAMICS**

Researchers: Jaroslav Koča, Igor Tvaroška, Petr Kulhánek, Stanislav Kozmon, Manju Kumari, Jakub Štěpán, Tomáš Trnka

Allocated computational resources: 2,000,000 core hours

Carbohydrates play a critical role in many biological processes. On cell surfaces, they often take the form of highly branched glycoconjugates. The synthesis of such glycoconjugates involves many enzymes. Disruption of these enzyme activities can lead to life-threatening pathological conditions such as diabetes, Alzheimer’s disease and cancer. The study aims to investigate the reaction mechanisms of these enzymes at the atomic level, which may aid e.g. in drug development.

**SIMULATIONS OF PARTICLE ACCELERATION BY SHORT ULTRA-INTENSE LASER PULSES**

Researchers: Onřej Klimo, Jan Pšikal, Jiří Vyskočil, Naveen Chandra Pathak, Martin Mašek, Tadzio Levato

Allocated computational resources: 650,000 core hours

The spatial and financial requirements of current particle accelerators considerably complicate their use in medicine, for example in cancer treatment. The main objective of this research is to understand how particle acceleration by high-intensity lasers operates. This research may contribute significantly to the development of future high-quality and less expensive sources of protons and X-rays from accelerated electron beams. These can be used for imaging very small structures on the order of nanometres (e.g. biological samples) and also for researching matter in astrophysics.

**IN SILICO DRUG DESIGN**

Researchers: Pavel Hobza, Pathik Brahmkshatriya, Jan Řezáč, Jindřich Fanfrlík, Martin Lepšík

Allocated computational resources: 200,000 core hours

Computer aided drug development has garnered a lot of attention due to its advantages, which include speed, low costs and the ability to select appropriate components for synthesis and subsequent biological screening. The aim of this project is to identify novel ligands that bind with therapeutically relevant proteins. Over the long term, the team has been researching components that are active in the treatment of cancer and acquired immunodeficiency syndrome (AIDS).

**FLOCON – A PROJECT BY THE AEROSPACE RESEARCH AND TEST ESTABLISHMENT**

Researchers: Petr Vrchota

Allocated computational resources: 100,000 core hours

The FloCon project is aimed at affecting the boundary layer on the wings of modern commercial aircraft through blowing. The objective is to improve aerodynamic performance and reduce environmental impacts. CFD models for simulating modern 3D active flow control technologies will be prepared, tested and validated and subsequently implemented into the aerodynamic optimization loop.
From May 27 to May 31 took place in Velké Karlovice the High Performance Computing in Science and Engineering 2013 conference. More than a hundred of participants from seven countries focused particularly on applied mathematics, numerical linear algebra, and optimization methods. The conference chair, Tomáš Kozubek, plans to organize the conference regularly every 2 or 3 years.

OLAF SCHENK, renowned expert on applied research in the field of HPC and Computational Science and author of successful PARDISO software from Università della Svizzera Italiana, also accepted our invitation. His cooperation with IT4Innovations National Supercomputing Center was started in the framework of a FP7 project EXA2CT.

Olaf Schenk: Three major achievements

1. PARDISO software, used by thousands of users: a thread-safe, high-performance, robust, memory efficient and easy to use software for solving large sparse symmetric and unsymmetric linear systems of equations on shared-memory and distributed-memory multiprocessors. The solver has been licensed to thousands of researchers at international scientific laboratories and universities since its first release in 2004.

2. Recipient of the Department of Energy’s 2013 Innovative and Novel Computational Impact of Theory and Experiment (INCITE) multi-year award totaling 100 million core hours on Oak Ridge National Laboratory’s Cray XK7 “Titan”. “Titan” is currently the fastest supercomputer in the USA with 17.59 petaflops and over a quarter of a million NVIDIA K20x accelerator cores and it will be used for research in the area of computational wave propagation.

3. Overview study on large scale diagonalization techniques for the Anderson Model of Localization, in which he in cooperation with Prof. Matthias Bollhöfer and Prof. Rudolf Römer showed that the problem regarded by some professionals as unsolvable, has a real solution. The study was awarded as the best article in SIAM Review in 2008.
How do you like our conference?
It’s been very nice; I like smaller events that enable intensive discussions. I am getting to know new colleagues, but also students from other universities and that is very inspiring. You can see in which way they think and what questions they deal with.

When did you hear first about IT4Innovations?
Frankly, it was only a couple of months ago. After all, IT4Innovations are launching their first supercomputer only now. However, I find important the fact that we immediately created a successful cooperation - it is the EXA2CT project, supported by the 7th Framework Programme. I regard that project, together with this conference, as a start of future collaboration with IT4Innovations. In the Czech Republic, there are two significant teams dealing with HPC. The first one - the Prague group around professor Tůma - is engaged in computational mathematics. Whereas the newly established IT4Innovations team is oriented also on fundamental research in HPC and Computational Sciences, and that is very good.

You are well-known for your achievements in technology transfer. This is also an important topic in the Czech Republic. Is there any formula for such success?
Well, of course you must have something to offer. But seriously - the easiest way is always to be contacted directly by the industry, when they make the first step. In order to make this happen, you must visit conferences, shake hands. Have prepared your theory, software, and of course the results. But the key thing is also the way you communicate. If you’re addressing the scientific community, your speech shall be different than if you’re addressing the industry. People from industry have different backgrounds; they often cannot extract from your research the things which might be useful for them. You must be able to highlight it yourself, to entice them. The mode of communication with industry is not better or worse than the mode of communication with scientific community, but it’s definitely different.

So, you mean a communication comprehensible for industry?
Yes, provided that you want to collaborate with industry. After some time it also helps referring to successful projects. Even for me, it is easier to establish contacts with industry after presenting Pardiso. They already know what work I am ready to do with my team. But this also has its drawbacks. Until now, it happens to me that some colleagues connect me with only this type of research because it’s the only one they know about.

How to motivate academia and industry towards a more intensive cooperation?
In Switzerland, the government supports the cooperation with special grants - 90% is paid by the government, and the remaining 10% must come from the industry. This is a very good way. If industry invests 10% into something, which is often a large sum of money, they must be confident that this collaboration is meaningful. However, this also comes with the motivating incentive of government funds. This is a perfect configuration ensuring a sufficient support of quality and viable projects.

Do you have any rules by which you select your industrial partners?
For me, the most important thing is the research topic and my role in it. As my specialization is on applied research, it is easier for me. But I must add that my involvement is practically the same, no matter if we are making research with an industrial partner or without it. I am still focusing on specific research tasks that interest me. But I have one condition - cooperation is conceivable for me only under condition that there are no implications limiting the publication of my research results. Everything developed by me and my colleagues must be publishable to the same extent as if it was developed without involvement of industry. Or I would not be able to enter such cooperation.

Would you like to express any wishes for the IT4Innovations supercomputing centre?
Certainly many other research projects like EXA2CT. It will also be important for the Czech supercomputing centre to consolidate and even to enlarge the user community in the long-term perspective. This is the biggest challenge not only for you, but also for other countries.
During the week of 17 to 21 June, IT4Innovations hosted the PRACE Summer School – Frameworks for Scientific Computing on Supercomputers. For five days, 50 participants from nine European countries were trained in the use of libraries and frameworks for supercomputers – libMesh, PETSc, Trilinos, Magma & Plasma, and Paraview.

PRACE Summer School 2013 in Ostrava was one of the PRACE seasonal schools that are held four times a year, each time in a different member state. Both the school’s topic and tutors are selected by the host organisation. The organizers managed to secure renowned lecturers from the USA, France and Germany, who are members of the development teams of the different libraries and frameworks that were presented. The tutorials also included hands-on exercises that took place on the new IT4Innovations system – Anselm.

The entire Summer School took place in the unique industrial setting of Dolní Vítkovice, literally in the shadow of blast furnaces. As part of the accompanying programme, the participants thus had the opportunity to learn about Ostrava’s history, which is closely connected with heavy industry, and climb up Blast Furnace 1 that is opened for visitors.

For feedback and suggestions, please contact us at klara.janouskova@vsb.cz