

newsletter



IT4Innovations
Centre of Excellence

Minister of Foreign Affairs Karel Schwarzenberg visited Supercomputing Centre IT4Innovations

The Minister of Foreign Affairs, Karel Schwarzenberg, opened his one day tour around Northern Moravia by visiting IT4Innovations. Accompanied by the rector of Technical University of Ostrava Ivo Vondrák and the director for strategic development of IT4Innovations Martin Duda he attended a presentation of applications that are prepared for the supercomputer, namely modeling of flooding and numerical modelling for engineering.



Ladies and gentlemen, dear colleagues,

Most likely, I am not alone feeling that this year has – yet again – been somewhat shorter than the previous one. This may be because a lot has been happening, including our IT4Innovations project.

First, I am glad that we have been increasingly successful in getting involved in research projects that are both interesting and, as I believe, useful regardless if it is in collaboration with the industry or the academic sector. For example, a year ago we made an agreement with DHI, a Danish company dealing with environmental simulations (and anything else environmental), to test the potential for mutual collaboration on a pilot project. A year later, we are at the stage where the company is ready to invest substantial financial resources in further joint application development. What is more, these applications are supposed to run on our future computational resources. We find ourselves working with an ever increasing number of serious candidates that are interested in using our future supercomputing capacities, such as the Biomedreg Centre of Excellence.

However, research achievements do not materialize out of thin air. Our scientists and IT experts have been doing an excellent job, but even that would not be enough. This year, there has also been a lot of hard work by everyone who is involved in ensuring that there will be something to work on in the future as well. Therefore, it is with great pleasure that I am able to inform you that we have handed over the construction site to the contractor that will build the supercomputing centre and we expect to sign a contract with the supplier of the small cluster (the initial portion of the supercomputer) by the end of the year. For more details, please read the next issue of the newsletter.

Let me take this opportunity to wish you good health and happiness in the New Year. I also wish that – in addition to online video broadcasts and simulation models – we will have more time to meet in person and more opportunity for “manual labour and rest”. Life is not just about supercomputing. Although...

prof. Ing. **Ivo Vondrák**, CSc.

Rector of VSB – Technical University of Ostrava



IT4 researcher wins Best Paper Award at world's most prestigious conference on membrane computing

A paper by Associate Professor Petr Sosík, a member of the IT4Innovations research team at Silesian University in Opava, received the Best Paper Award at the 13th annual global conference on membrane computing that was held in Budapest. He received the award for his paper entitled "Limits of the Power of Tissue P Systems with Cell Division".

The paper addresses information exchange in organisms – using mathematical models (membrane systems), it studies the exchange of information of molecules through cell membranes. Associate Professor Sosík demonstrates that interconnected systems of proliferating cells are able to solve equally difficult problems that modern parallel computers are. His research brings together different areas of science and his perspective as an IT scientist to help to understand how nature can deal with information.



Associate Professor Sosík comments on his success. "I greatly appreciate the award, as the conference is attended by the most prominent scientists in this field." While the results of membrane computing research are also presented at a number of other international scientific forums, this is the only conference that is focused exclusively on this field. Even though the conference attracts attendees from all over the world, the core of the research remains in Europe.



The 1st IT4Innovations Annual Conference

The first annual conference of the IT4Innovations Research Centre took place on 22 and 23 October 2012. Representatives of

research programmes and project partners presented their current results and outlined the main focus of their research.



HiPEAC membership to extend collaboration with European research centres



Through Director Martin Palkovič, IT4Innovations became a member of HiPEAC (the European Network of Excellence on High Performance and Embedded Architecture and Compilation), a European network of research centres financed by the 7th Framework Programme. The goal of the HiPEAC network is to strengthen the European research community in computing systems, by gathering the leading European academic and industrial groups.

The HiPEAC network is based on personal collaboration. It brings together leaders of both academic institutions and industrial R&D groups. Under the umbrella of a joint virtual centre of excellence, it allows them to collaborate on joint research projects. "Through HiPEAC, we can shape the future of computing systems in Europe," commented Martin Palkovič.

The HiPEAC network coordinates working groups that are composed of members and partners from different countries and address joint research tasks. Furthermore, HiPEAC organizes a wide range of conferences, internships, seminars and summer schools and publishes newsletters to share information. These are available to all members and their parent organizations.



PRACE computational resources awarded to **6 projects** from the Czech Republic



Following last year's success of Associate Professor René Kalus's team, five additional research projects from the Czech Republic have succeeded in competing for PRACE computational resources within PRACE Preparatory Access. All of the projects were submitted by IT4Innovations experts. Overall, they obtained nearly 31.5 million core hours on machines throughout Europe. In financial terms, the success is worth tens of millions of Czech crowns. The computational resources acquired will be used to pursue long-term research objectives in molecular simulation and the development of scalable algorithms in engineering.

THE MODELLING OF THE THERMODYNAMIC AND STRUCTURAL PROPERTIES OF WATER MOLECULE CLUSTERS

Examples of supported PRACE projects:

Researchers: **Aleš Vítek, Martin Stachoň, René Kalus**

The project focuses on the modelling of the thermodynamic and structural properties of small clusters of several to tens of water molecules. While many theoretical studies on thermodynamic properties have been published over the past two decades, almost all of them addressed the case where there is constant volume and temperature, i.e. volume and energy. Only a few studies have addressed the behaviour of molecule clusters at non-zero pressure. This project aims to fill that gap. The output will consist of complete phase $p - T$ diagrams. Overall, they acquired the opportunity to use Tier-1 systems for 2 352 000 core hours.

DOUBLE SUCCESS FOR FETI METHODS FROM THE DEPARTMENT OF APPLIED MATHEMATICS

Researchers: **David Horák, Václav Hapla, Michal Merta, Martin Menšík**

'FETI' methods are among the most successful methods for the parallel solving of large-scale engineering tasks. They allow for dividing the computational area (e.g. a car engine model, a mine support model etc.) into a predetermined number of sub-areas, each of which is then assigned to one processor. This 'division of labour' not only speeds up calculations in direct proportion to the number of computing cores used, but also allows for calculating much larger tasks since the memory of a single computer no longer poses a limit. Another advantage of FETI methods is the possibility of 'dualization' where the entire task is converted to the boundary between the different sub-areas. In doing so, we can considerably reduce the number of unknowns and obtain a problem that is easier to solve.

This group primarily focuses on using the 'Total-FETI' method that has been developed by the Department of Applied Mathematics at VSB - The Technical University of Ostrava. When combined with scalable algorithms that are being developed by Professor Dostál's group, the method can also be used for other needs, such as the parallel solving of contact tasks between two or more objects. Reliable solutions to such problems are of great practical use in engineering. Our FLLOP library is able to utilize thousands of computing cores to solve tasks with tens of millions of unknowns. The main objectives of the projects are to test the library on real-life engineering problems and optimize it, as well as to find the best strategy for a scalable solution for tasks with hundreds of millions of unknowns.

Courtesy of the HPC-Europa2 and PRACE-DECI projects, we are currently using mainly the Hector supercomputer, which is located in the UK and has more than 90 000 computing cores. As a part of PRACE Preparatory Access, we have also gained access to Europe's most powerful supercomputers, namely Curie in France and Hermit in Germany.

RESEARCH OF THE ELECTRON CLOUDS OF INERT-GAS ATOM CLUSTERS THROUGH SUPERCOMPUTER SIMULATIONS

Researchers: **René Kalus, Martin Stachoň, Aleš Vítek, Ivan Janeček**

Another success is the 16 000 000 hours of computing time on the Hermit supercomputer (HLRS, Stuttgart) for simulating the electron clouds of inert-gas atom clusters. This project is part of the basic research on the behaviour of these systems and has potential for use in practical applications, for example in medicine. For illustration, if we wanted to perform these calculations (which are based on the rules of quantum physics) on VSB-TUO's currently most powerful computer, this would take anywhere between ten and fifteen years.

This complex research is aimed at developing methods that would make it possible to study collision processes, including electron excitations. In the near future, these methods could allow for the realistic modelling of systems such as helium plasma, which is highly effective in sterilizing surgical and other medical instruments, or even wounds.

We would appreciate it if you sent us your feedback and suggestions to klara.janouskova@vsb.cz

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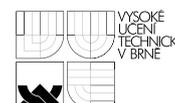
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