IT4INNOVATIONS

DIGITAL INNOVATION HUB


IT4Innovations
IT4Innova

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

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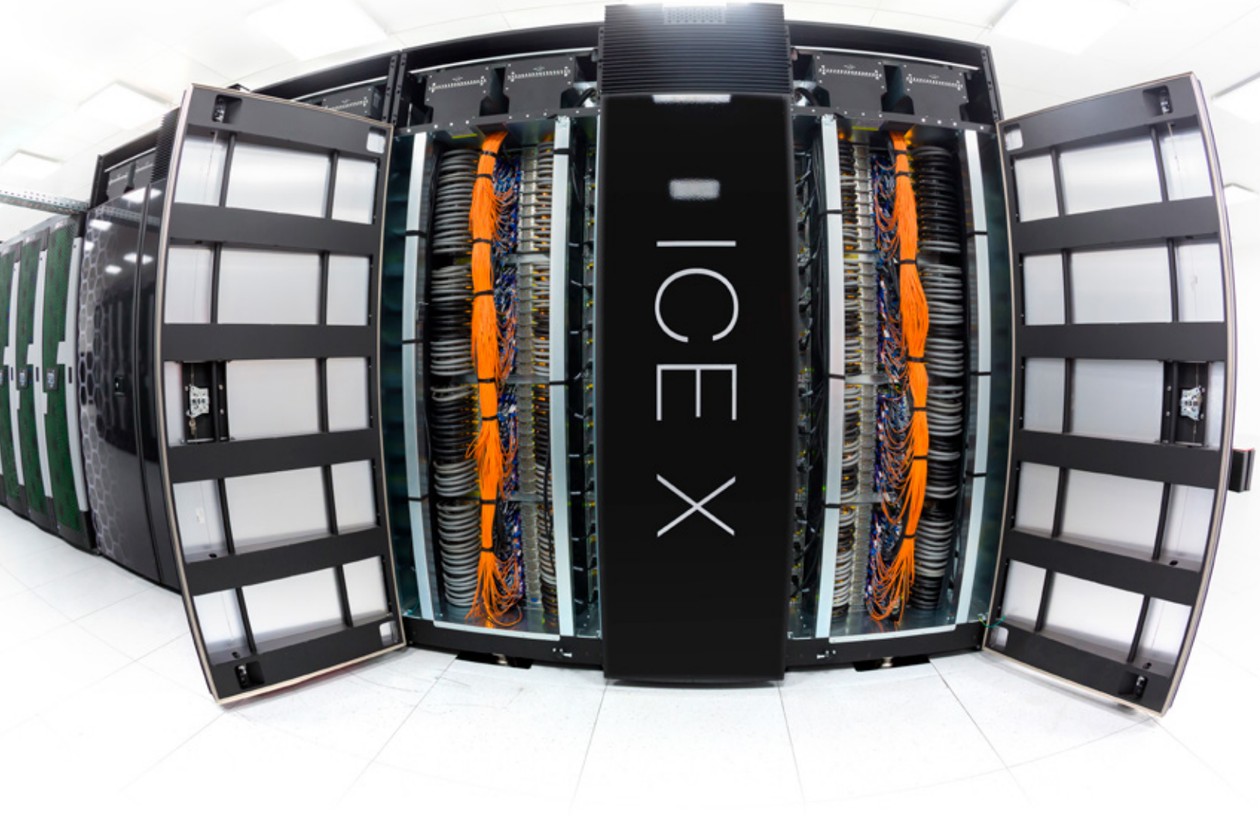
DIGITAL INNOVATION HUB

Editors: Tomáš Kozubek, Tomáš Brzobohatý



Dear reader,

Today supercomputers have already been deemed tools of unquestionable importance in assisting science. However, with their capacity to manage highly demanding computations and process enormous amounts of data, they are increasingly used across various industries such as mechanical engineering, civil engineering, the energy industry, the health sector, transport, and natural disaster management. Therefore, IT4Innovations National Supercomputing Center aims to fulfill its mission of aiding the digitalization of the Czech community and its industry via supercomputing infrastructure and relevant know-how. In the field of industry in particular, IT4Innovations aims to involve Czech companies in the domains of High Performance Computing (HPC), artificial intelligence, and big data analysis, demonstrating how supercomputers can help them as well. In this publication, you can find several examples of our successful cooperation with small, medium, and large enterprises, all of whom have taken advantage of our services. There are various options and levels of cooperation with us: from simple rental of computational resources to complex generation of solutions for a particular problem, which includes research, and development of computer code along with its deployment on our supercomputing infrastructure.

During the seven years of our existence, we have joined several international initiatives, consortia, and projects, which contribute to supercomputing technology development. The very first such involvement has been in the ongoing pan-European Partnership for Advanced Computing in Europe (PRACE) research infrastructure. Additionally, we also joined the European Technology Platform for High Performance Computing (ETP4HPC), which is focused on defining research and technology priorities in the field of high-performance computing. Our involvement in the field of algorithms development and code optimization has been appreciated by the Intel company, who have made us a member of the Intel Parallel Computing Center group, a prestigious selection of research institutions and supercomputing centres worldwide.

Moreover, we have become an important centre for education in HPC. We are proud to be one of the PRACE Training Centres, offering a comprehensive training programme. We have also established a brand new Computational Sciences PhD study programme. It is precisely educational activities above all which are at the centre of our focus, as successful deployment of HPC and all digital technologies, in general, in industrial practice, and in daily life is critically dependent on the availability of sufficient human resources endowed with corresponding expert knowledge.

The European Commission has recognized our industrial partners-focused activities by awarding us the status of a successfully operating Digital Innovation Hub (DIH) in the field of high performance computing, artificial intelligence, and advanced data analysis. We are a member of consortia for several international projects, the objectives of which are to assist small and medium-sized enterprises in overcoming the obstacles in accessing and using supercomputers for their own innovations and development. The projects include SESAME NET, InnoHPC, CloudiFacturing, TETRAMAX, and POP 2 Centre of Excellence, as well as the pan-European PRACE-based programme supporting HPC adoption by small and medium enterprises called the SME HPC Adoption Programme in Europe (SHAPE).

I believe that this publication will ignite inspiration, and together we will pioneer new ways for HPC to help develop businesses, including yours.

VÍT VONDRÁK
IT4Innovations Managing Director

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ABOUT IT4INNOVATIONS

IT4Innovations National Supercomputing Center, a university institute at VŠB – Technical University of Ostrava, assures the operationality of the most powerful supercomputing technology in the Czech Republic. With respect to its uniqueness and significance, it ranks highest among large national research infrastructures of the Czech Republic. It is currently operating two powerful supercomputers – Anselm and Salomon, the latter of which still ranks among the top European supercomputers. IT4Innovations is also a research and development centre with strong international links and as such, it is currently involved in good number of international projects funded primarily by the Horizon 2020 programme. Since its foundation in 2011, IT4Innovations has been a member of the prestigious pan-European PRACE (Partnership for Advanced Computing in Europe) research infrastructure, where it represents the Czech Republic. Since 2016, it has also been involved in the European Technology Platform for High-Performance Computing (ETP4HPC), which focuses on defining technology and research priorities in the field of high-performance computing in Europe. For its activities focused on supporting the deployment of computationally intensive numerical simulations and advanced data analysis primarily in small and medium-sized enterprises, IT4Innovations is registered by the European Commission as a Digital Innovation Hub in the fields of HPC, artificial intelligence, and advanced data analysis.

http://s3platform.jrc.ec.europa.eu

Since the beginning of the year 2018, IT4Innovations has also been participating in the preparation of the EuroHPC joint undertaking in cooperation with other European countries, the objective of which is to support the construction of a European exascale supercomputer by 2022/2023 and thus significantly contribute to digitalization of the European community and industry.

Mission of IT4I

The mission of IT4Innovations is to conduct excellent research in the field of high-performance computing and data analysis, run a leading national supercomputing infrastructure, and mediate its efficient utilization to increase the competitiveness and innovativeness of Czech science and industry.

Vision of IT4I

IT4Innovations aims to become a top supercomputing centre providing professional services and conducting excellent research in the fields of high performance computing and big data processing for the benefit of science, industry, and the entire community.

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ABOUT THE DIGITAL INNOVATION HUB

The Digital Innovation Hub (DIH) represents a support instrument, the objective of which is to assist companies in increasing their competitiveness by means of digital technologies improving their business/production processes, products, and services. DIHs act as one-stop-shops helping companies integrate digital technologies into their business activities.

Digital Innovation Hubs provide access to knowledge and technologies not commonly available to companies, who are thus given an opportunity to experiment with these digital innovations. This will considerably simplify decision making and subsequent implementation of these technologies and know-how in company structures. The key clients of these DIHs include small and medium-sized enterprises, as well as public administration and healthcare institutions, which help to enhance the quality of community life by implementing digital innovations.

Moreover, Digital Innovation Hubs also provide a space where important players in the field of digital innovation development can meet and connect. They include, among others, the connection of start-ups with investors, the preparation and education of potential users of these innovations, support of their use along with other key technologies, and other areas of economy and society.

Digital Innovation Hubs offer not only technological skills and business development knowledge but also provide independent expert opinion. In order to put digital skills into practice, technological know-how is indisputably an essential condition, but clearly not a sufficient one. No less important is to know how to define specific the needs of companies, which can be met by implementing the above-mentioned digital solutions. Ideally, entirely new opportunities, resulting in the need for, and implementation of completely new business models as well as leading to a brand new strategic direction for a company, might arise.

IT4Innovations Digital Innovation Hub aims to fully realize the above-mentioned definition. In this context, a key partnership of IT4Innovations and the Moravian-Silesian Innovation Centre Ostrava (MSIC) is being established. These two institutes are expert centres possessing their own specific know-how.

DIGITAL INNOVATION HUB

Business development and support

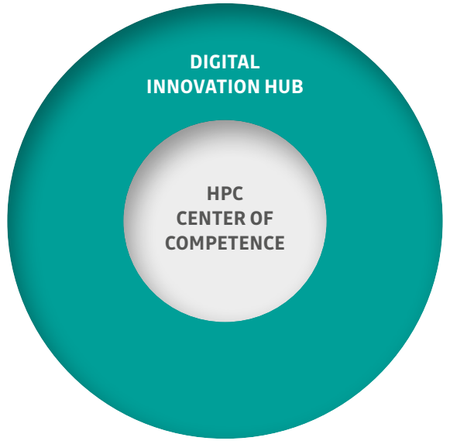
Incubator/mentoring services

Market intelligence

Innovation ecosystems

Brokerage

Access to finance



CENTER OF COMPETENCE

HPC and data infrastructure

HPC and HPDA adoption programme

Applications

Code optimization

Skills and best practices

User support

Training

IT4Innovations
Digital Innovation Hub scheme

IT4Innovations specialises in providing High Performance Computing (HPC) services, computer simulations and modelling, advanced data analysis, augmented and virtual reality, and artificial intelligence. The main focus is on possible uses of supercomputing technologies within the HPC Competence Centre, which is being developed in this perspective.

One of the key activities of MSIC is to provide individual business consulting services to facilitate the introduction and development of innovation in companies. These services are focused not only on the foundation and growth phase of new start-ups but also on supporting the dynamic development of already established companies. Within the DIH, MSIC will primarily provide services in areas such as business development, mentoring, networking, and ensuring funding for new technologies to companies.

Integration of the know-how of both organizations thus creates a unique opportunity to provide a full portfolio of attractive and complementary services to companies in one single place (a one-stop-shop).

The main concept of the Digital Innovation Hubs network is based on the principle of the proximity of DIHs to their clients. From this perspective, the primary clients for IT4Innovations DIH are companies based in the Moravian-Silesian region. However, the expertise and technologies of this hub present assets the value and potential use of which go beyond the borders of both the region and the Czech Republic. Moreover, representatives of the IT4Innovations DIH are currently actively involved in the debate and activities associated with defining the co-operation (including task distribution) among the DIHs within the Czech Republic as well as at the EU level. In this regard, this "Ostrava hub" is carefully preparing to play an important role in fulfilling the vision of the Digital Czech Republic as well as Digital Europe.

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THE INFRASTRUCTURE

In June 2013, our ANSELM supercomputer with a theoretical peak performance of 94 Tflop/s became operational, followed by the Salomon supercomputer with a theoretical peak performance of 2011 Tflop/s two years later. At the time it became operational, Salomon ranked 40th in the TOP500 list of the most powerful supercomputers in the world. Salomon is the most powerful European system based on the first commercially available generation of Intel Xeon Phi (Knights Corner) co-processors. At the beginning of the year 2019, a new system with an approximate theoretical peak performance of 800 Tflop/s is planned to support our current supercomputers. This new system is to be equipped with the latest available technology including processors with the AVX-512 instruction set, Nvidia Tesla V100 accelerators, a fat compute node with a memory of up to 6 TB, 200 Gb/s interconnect, NVMe memory--based storage, and BurstBuffer technology for accelerating data access. For the field of artificial intelligence and machine learning, we plan to buy specialized NVIDIA DGX-2 hardware at the beginning of 2019, which is highly optimized for such problems.

All our supercomputers are located in the data room of IT4Innovations National Supercomputing Center situated within the VŠB – Technical University of Ostrava campus. The data room, with an area of about 500 m^2, is equipped with an elevated floor, underneath which is enough space for the power supply system, and inlet and outlet of the warm water (30 °C – 55 °C) and cold water (6 °C – 28 °C) supply equipped with valves for easy connection of water-cooled racks. The data room is equipped with a fire protection system based on active reduction of the oxygen concentration to a level of about 15 %, which physically prevents a fire from starting and spreading. The computer systems operation is sustained by up to 2,5 MW of fully redundant power input capacity backed up by our own diesel generators as well as about 500 kW of cooling capacity produced by a system of redundant cooling circuits including 15 cooling towers. Part of the data room is also comprised of redundant data connections to the national CESNET network as well as to the Internet.

Technical parameters of the IT4Innovations computer systems

	ANSELM	SALOMON	New system
Put into Operation	Spring 2013	Summer 2015	Projection - 2019
Theoretical Peak Performance	94 Tflop/s	2011 Tflop/s	>800 TFlop/s
Operating System	RedHat Linux 64bit 6.x	RedHat Linux 64bit 6.x, CentOS 64bit 6.x	Linux
Compute Nodes	209	1008	198
CPU	2x Intel SandyBridge, 8 cores, 2.3 / 2.4 GHz, 3344 cores in total	2x Intel Haswell, 12 cores, 2.5 GHz, 24192 in total	2x Intel Cascade Lake, 18 cores, 2.6 GHz
RAM	64 GB / 96 GB / 512 GB	128 GB / 3.25 TB (UV compute node)	192 GB / 6 TB (fat compute node)
GPU Accelerators	23x NVIDIA Tesla K20 (Kepler)	N/A	32x NVIDIA Tesla V100 (Volta)
MIC Accelerators	4x Intel Xeon Phi 5110P	864x Intel Xeon Phi 7120P, 61 cores each, in total 52704 cores,	N/A
Disk Storage	320 TiB / home (2 GB/s), 146 TiB / scratch (6 GB/s)	500 TiB / home (6 GB/s), 1638 TiB / scratch (30 GB/s)	25 TiB / home, 200 TiB / scratch (30 GB/s)
Interconnect	Infiniband QDR 40 Gb/s	Infiniband FDR 56 Gb/s	Infiniband HDR 200 Gb/s

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INFORMATION SECURITY

Since December 2018, IT4Innovations National Supercomputing Center has been an Information Security Management System certificate holder according to the international **ISO/IEC 27001:2013 (Czech version: ČSN ISO/IEC 27001:2014) standard.**

The ISO 27001 certificate has been awarded for the following areas:

- provision of national supercomputing infrastructure services
- high-performance computing problems solutions
- performance of advanced data analysis and simulations
- processing of large data sets

Certification according to this standard based on the PDCA cyclic method principle certifies that IT4Innovations plans, maintains, evaluates, and continually improves its information security management system. In the field of information security, it includes continual risk management, defining security policies, evaluating the efficiency of adopted measures, mitigating potential impacts, raising the security awareness of employees, managing interactions with economic operators, and securing other security aspects at the organisational and administrative, personal, physical, and cryptographic levels.

The awarded certification is valid in the context of all organisational units; institutional departments and all employees. Information security is thus managed not only in the area of operation and provision of information technologies but also science, research, and administration.

This certification is subject to regular independent audit, which is performed by a certification body accredited by the Czech Accreditation Institute, a public-benefit non-profit organization. IT4Innovations thereby demonstrates that ensuring information security of all interested parties is part of its strategic security vision.


TDS Brno - Sekce řízení jakosti a certifikace, p. s.
U vlečky 29/5, 617 00 Brno
Certification body for management systems no. 3105
accredited by the Czech Accreditation Institute according to ISO/IEC 17021-1:2015

CERTIFICATE
No. TDS 81/2018

The TDS CERT
certification body
for management systems

confirms

on the basis of a positive result of certification audit No. 315/2018,
that the company

VSB – Technical University of Ostrava
IT4Innovations National Supercomputing Center
17. listopadu 2172/15
CZ - 708 00 Ostrava

has established and applies an information security management system
in accordance with

ISO/IEC 27001:2013

in the line of

Provision of national supercomputing infrastructure services, solution of computationally intensive problems, performance of advanced data analysis and simulations, and processing of large data sets.

Statement of Applicability ver. 01 – 07/12/2018.

This certificate is valid until 12th December 2021.

Further explanation as to the subject and certificate as well as to applicability of requirements referring to Standard ISO/IEC 27001:2013 can be obtained at the indicated organization

Brno, 13.12.2018

S 3105

Ing. Jiří Noss
Director of certification body

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OUR PORTFOLIO OF SERVICES

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COMPUTATIONALLY INTENSIVE MODELLING AND SIMULATIONS

IT4Innovations National Supercomputing Center offers its industrial partners many years of experience with computationally intensive numerical simulations and virtual prototyping. We can perform customized simulations of physical processes related to fluid flow, structural mechanics, heat transfer, acoustics, and electromagnetism. The IT4Innovations researchers have complex expertise in applying both commercial software packages, such as ANSYS Multiphysics, Fluent, CFX, Comsol Multiphysics, MSC Marc, and LS-DYNA, and non-commercial open source packages, such as OpenFOAM, Code_Saturne, Code_Aster, Elmer, and Calculix.

Structural mechanics

- modal analysis of constructions with calculation of natural frequencies and vibrational modes
- harmonic analysis, amplitude-frequency response to harmonic and random waveform excitation
- dynamics of rotor systems
- nonlinear harmonic balance response
- linear and nonlinear static analysis of systems with geometric and material nonlinearities, contact problems, plasticity, hyperelasticity, viscoplasticity
- dynamics of complex systems – implicit/explicit dynamics
- simulation of fast phenomena – crash tests/ drop tests
- evaluation of marginal states related to material cohesion failure

Heat transfer

- linear and nonlinear heat transfer
- steady states and time-dependent problems
- diffuse radiation, solar radiation
- heat transfer in contact interface
- phase transition/solidification

Flow simulation - CFD

- steady state and time-dependent fluid flow solutions
- incompressible/compressible flow
- turbulent flow - RANS/LES/DES
- moving meshes, mesh morphing
- multiphase flow
- combustion

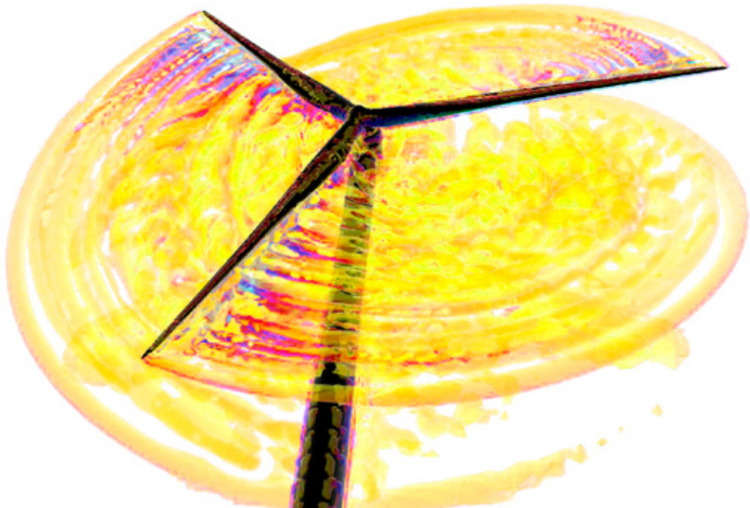
Sound wave propagation

- aeroacoustics, vibro-acoustics
- harmonic sound wave propagation
- time-dependent simulation of sound wave propagation

Multiphysical problems

- thermal-structural problems
- CFD–flow, heat, radiation, chemical processes
- FSI – fluid structure interaction

Shape and Topology Optimization



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ADVANCED DATA ANALYSIS AND SIMULATIONS

In the field of advanced data analysis and simulations, IT4Innovations is engaged in big data processing and analysis as well as simulations for various practical applications. They include, for example, support for management and decision making in emergency situations, smart navigation, traffic load prediction, flood propagation modelling, smart cities, bioinformatics, and reliability analysis. Moreover, we are involved in the field of programming models for distributed applications and their efficient implementation.

Smart City and traffic modelling

- implementation and modification of algorithms for traffic modelling
- global approach to transport infrastructure
- smart navigation
- urban traffic flow management
- optimization problems: optimization of distribution/collection of goods to customers
- interaction of traffic modelling with other topical areas (floods, pollution)

Production and inventory management

- efficient material flow management
- sales prediction based on sales history data
- inventory optimization
- statistical methods for time-series analysis

Crisis/Emergency management support: Floreon+

- hydrological monitoring and modelling
- monitoring of current traffic situation
- modelling of dangerous substances discharge
- population mobility monitoring
- detection of soil movements
- modelling of crisis situations interactions

Bioinformatics

- genomics and molecular diagnostics in cooperation with professionals from the health sector and academia
- development and testing of bioinformatics tools
- interfaces for accessing the computing infrastructure

Radar Earth observation

- identification of landslide activity
- monitoring of vertical movements of structures
- mapping of inundated areas through clouds
- evaluation of vegetation changes such as deforestation

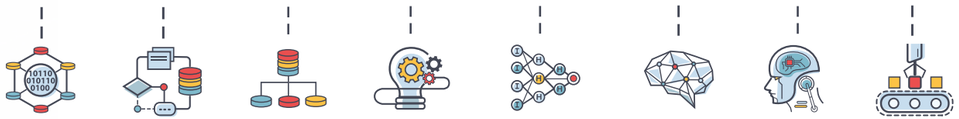
Bioimage analysis

- processing of large bioimage datasets
- parallelization of light sheet microscopy data processing
- extending the FIJI platform for bioimage data analysis with a module for processing of data using HPC

MRI/CT data processing

- reconstruction of 3D models of tissues via processing of Magnetic Resonance and Computed Tomography-generated data
- in-house software tools for image reconstruction developed in cooperation with University Hospital Ostrava

MACHINE LEARNING



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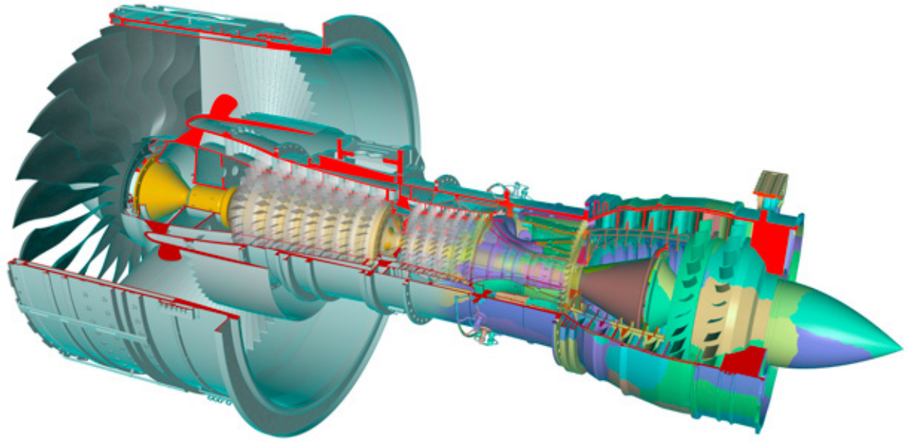
DEVELOPMENT AND IMPLEMENTATION OF FEM/BEM SIMULATION TOOLS



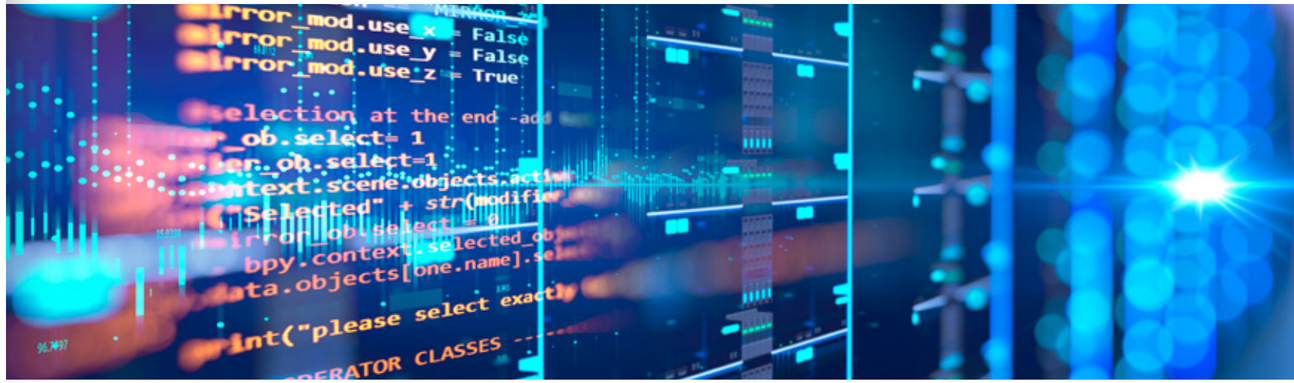
We offer our knowledge and experience with developing and implementing new efficient methods for computationally intensive numerical simulations in mechanical engineering, civil engineering, the energy industry, and biomechanics. IT4Innovations develops its own in-house massively parallel open-source simulation tool ESPRESO, based on the finite element method for efficient utilization of the available HPC infrastructure. The free license for the use of this continually developing package allows fully automated simulation chains to be created. The added value of this package includes a massively scalable solver based on domain decomposition methods, which allows computational resources of currently the most powerful supercomputers to be fully saturated, and thus complex multiphysical problems to be solved.

Furthermore, we can create automated, customized computing tools based on open-source third-party products such as OpenFOAM, Code_Saturne, Code_Aster, Elmer, and Calculix. Apart from performing computations, we can also provide HPC technology-focused technical and expert support for all of the above-mentioned products.

ASSISTANCE IN DEPLOYMENT OF EXISTING CODES ON HPC SYSTEMS AND THEIR OPTIMIZATION

We provide assistance in deployment of existing codes on the HPC systems of both IT4Innovations and our partners. Within the scope of this support, we are able to assist with profiling of given codes and their possible optimization. Since 2018, IT4Innovations has been a member of the H2020 programme funded POP2 (Performance Optimization and Productivity) Centre of Excellence project, which is primarily focused on providing assistance with analysis of parallel applications, identification of bugs in codes, and recommendation of optimization methods, leading to higher performance and better scalability of a given application. Within the implementation period of this project, we provide our services free of charge to both academic and research institutions as well as to commercial companies established in EU. For a detailed portfolio of services, please visit the following project website:

https://pop-coe.eu/services



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RENTAL OF IT4INNOVATIONS COMPUTATIONAL RESOURCES

IT4Innovations offers commercial companies the opportunity to rent the computational resources of the operated supercomputers. Companies interested in using this service may choose based on their preferences from the following modes:

Standard allocation arranged for a specific period with a pre-agreed quota

This is essentially a rental mode based on shared access to computational resources with other active users, with a total number of core hours negotiated in advance, and includes the provision of standard user support.

Customized allocation

A rental mode offering the opportunity, for example, to use a pre-agreed number of compute nodes arranged for a certain period allowing instant access to computational resources as compared to the standard allocation.

Upon submission of an Application for Renting Computational Resources, the customer is presented with a draft Contract for Renting Computational Resources including securing the requisite consent of the provider (MEYS CR). Upon its receipt (usually up to 14 days), the customer obtains the Contract for Renting Computational Resources for signature. The customer is provided access to the computational resources at the latest within a period of 3 working days from the date of entry into force of the respective contractual relationship. The price per core hour for the year 2019 within the Standard allocation mode is EUR 0.046 (excluding VAT).

The use of computational resources within the rental is measured in core hours, which means that 1 CPU core is allocated for 1 hour.

General Terms and Conditions for renting computational resources on the computer system for high-performance computing

Technically, the customer's access to the systems is provided remotely using access servers. Allocation of computational resources and running and managing tasks are executed via the PBS Professional workload manager. The customer has the option to continually monitor the amount of core hours used, and is provided the standard user support. For a detailed manual for access to the cluster including technical and other requirements, please see the documentation for Salomon and Anselm clusters in the following link

https://docs.it4i.cz/

The Application for Renting Computational Resources shall include the following specifications:

- rental form,
- number of core hours,
- rental period,
- purpose of the rental,
- company information (customer´s business name, registered office, Company Registration Number, VAT Registration Number).

An example of renting computational resources

Cooperation based on renting IT4Innovations computational resources was established, for example, with the Forest Management Institute, a state-owned enterprise. This institute has used the IT4Innovations HPC technology for complex calculations of the Czech forest cover and forest change monitoring via satellite using Earth observation data. For this purpose, freely available data from the EU funded Copernicus programme, namely the Sentinel-1 and Sentinel-2 satellite data. IT4Innovations experts have also cooperated in the development of new algorithms to be used in the field of forestry.

Marek Mlčoušek

Forest Management Institute

Our cooperation with IT4Innovations plays a key role for us – without having the access to the HPC resources provided by IT4I, we would not be able to perform one of our activities, namely the evaluation of forest health and development using Earth observation data generated via remote-sensing technologies. We secure this activity periodically for the whole territory of the Czech Republic. In this context, computationally-intensive tasks, such as atmospheric corrections of all the Sentinel-2 satellite-generated data, subsequent automated generation of cloud-free scenes for the whole territory of the Czech Republic, and others, need to be solved. These are the types of tasks requiring big data approach, which cannot be applied on a nation-wide basis using standard desktop computers. Another positive feature that can also be considered is IT4I's helpful approach and highly qualified support provided in the first year of our methodology development, which allowed us to implement our solution within a research project.

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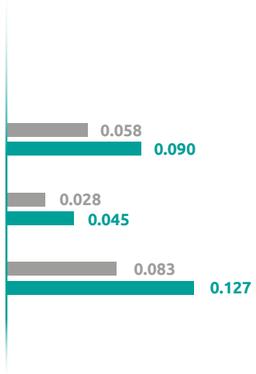
RENDERING

With reference to the opportunity to rent computational resources, IT4Innovations offers external partners 3D scenes rendering services. Rendering is performed using an extension of the open-source Blender software that supports two computing modes. The first mode is based on rendering via a standard CPU architecture, and the second one combines the Intel Xeon Phi (MIC) accelerators for rendering with one CPU used for pre-processing and post-processing. The second mode, in comparison with the standard approach using only the standard CPU architecture, is roughly half the price; however, there is scene size limit as it must go into the limited MIC memory.

Price comparison of both options using typical benchmark scenes.

Prices are listed in EUR excluding VAT



1/ **CLASSROOM**
by Christophe Seux

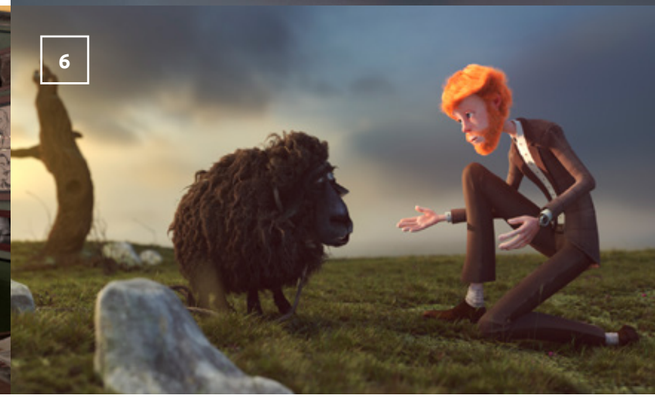
2/ **FISHY CAT**
by Manu Jarvinen

3/ **BARBERSHOP**
CC-BY-SA, Blender Institute, based on Agent 327 comics © Martin Lodewijk

4/ **PABELLON BARCELONA**
by Claudio Andres

5/ **BMW BENCHMARK**
from Mike Pan

6/ **VICTOR**
CC-BY, from the Gooseberry open movie project



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COLLABORATION EXAMPLES

CRANIAL REMOULDING ORTHOSIS DEVELOPMENT

Partner: **Invent Medical Group s.r.o. (IMG)**

Field: medical equipment and technology

State-of-the-art 3D scanning technology is used to achieve the best possible results.

In some new-borns, particularly those born prematurely, skull deformities may occur in the first few months of their life. The standard medical treatment in these cases includes using plastic cranial orthoses. Apart from being relatively heavy, unattractive, and airtight, these orthoses need to be adjusted during the treatment so as to "grow" along with a child's head. These adjustments as well as the initial production are enormously time-consuming, and uncomfortable for paediatric patients.

Invent Medical Group s.r.o. is a start-up company involved in the design and production of cranial orthoses using 3D printing technology. These orthoses are geometrically and functionally very complex, and their development is currently dependent on the experience of designers and health professionals.

The cooperation between IT4Innovations and IMG aims to automate many of these manual procedures making the whole process simpler and faster. Within the contract research projects, we focus on developing algorithms for automatic adjustment of cranial orthoses, application of optimization algorithms for finding the optimal head shape, and the use of numerical modelling methods for determining the orthosis stiffness. To guarantee the full functionality of orthoses it is necessary to determine their stiffness accurately, as this property critically affects the growth of a child's head to its desired shape. This stiffness is currently tested in the IMG laboratory using special devices. Testing must be performed for every new type of cranial orthosis, which makes its design considerably time-consuming and financially intensive. Within the cooperation between IT4Innovations and IMG, the laboratory experimental testing of orthoses has been replaced by numerical modelling methods using a supercomputer. The geometric model developed by the designers is automatically converted into a numerical model, which allows the orthosis deformation to be calculated for the required load. Based on these calculations, the final design is adjusted to fulfil the stiffness requirements, and the individual designs might also be compared.

Jiří Rosický

Invent Medical Group s.r.o.

Our cooperation with IT4Innovations is highly beneficial for our company. We are confident when we say that our field – custom-made orthotics and prosthetics – will not evade the emerging technology trends, among which the most important ones for us are digitalization and automation of the design and production processes. With IT4Innovations National Supercomputing Center, we are working on several projects – automation and optimization of CAD processes, computer simulation of stress-strain states, and development of custom-made software for clinical applications.

At the very beginning, we really clicked with IT4I – we are happy to be cooperating with this top-notch institution, which not only has an excellent technical background but also a team of genuine and keen experts. We believe that thanks to the new solutions developed within our cooperation with IT4Innovations our company is likely to become a global leader in the digitalization era of custom-made orthotics and prosthetics. We really appreciate the colleagues from IT4Innovations and those who made the foundation and development of this institution possible.

Orthoses are produced using 3D printing technology.

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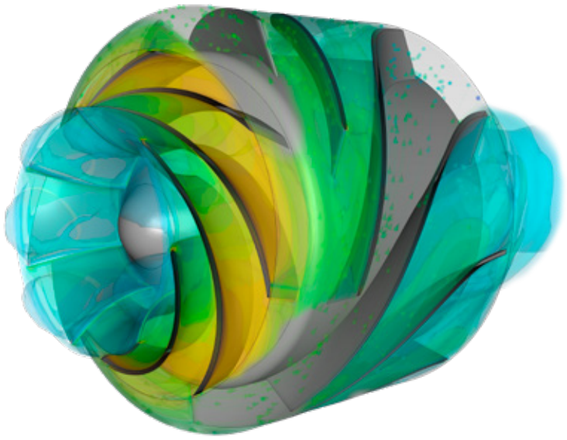
PUMP EFFICIENCY OPTIMIZATION USING OPEN SOURCE SOLUTIONS AND HPC

Partner: **SIGMA GROUP a.s.**

Field: mechanical engineering



In cooperation with the members of SIGMA GROUP a.s., a modern and dynamically expanding engineering company and the leader of the pumping technology market in the Czech Republic, we are aiming at making the optimization of bladed machines, such as centrifugal pumps, faster and cheaper. In centrifugal pump design, one of the most important parameters is their efficiency, which largely depends on the shape of the rotor and stator blades, and the geometry of the leading and trailing edges. In order to find the optimal shape of the above-mentioned part so the pumps reach the highest possible efficiency for a wide range of operating conditions, a large number of computationally intensive CFD simulations must be performed. The number of these simulations is closely linked to the number of design variables affecting the complex changes in the pump's geometry.

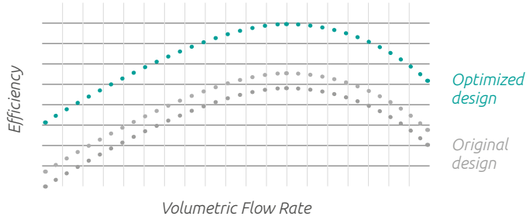
Using several hundred compute cores, the results of CFD simulation for one selected configuration of design variables, i.e. one fixed pump geometry, can be obtained within 0.5 to 2 days depending on the problem size and number of compute cores used. When a standard workstation is used, the computation time needed for one model may take as long as several weeks. Therefore, complex pump optimization becomes unfeasible in such a case. The IT4Innovations infrastructure provides sufficient computational resources allowing independent parallel running of computations of a large number of geometric models, thus reducing the time needed for finding an optimal solution to several days or weeks instead of months or even years in the case of using a standard workstation with limited computing power.

A standard established approach to pump optimization is the use of commercial tools for performing CFD simulations. When deployed on HPC infrastructure, their use becomes economically inviable due to the excessive financial costs of licence acquisition and the limited potential for adapting to customer needs.

The main objective of the joint activities is to replace the commercial solution with available open source libraries and their combination with the in-house software solution, which fully meets the requirements of the partner without any additional financial costs incurred by acquiring commercial licences. This solution in combination with the IT4Innovations HPC infrastructure allows the industrial partner to streamline the process of new machine design and thereby reduce the cost of the design cycle.

Time reduction of 98%
achieved by means of HPC as
opposed to a standard workstation

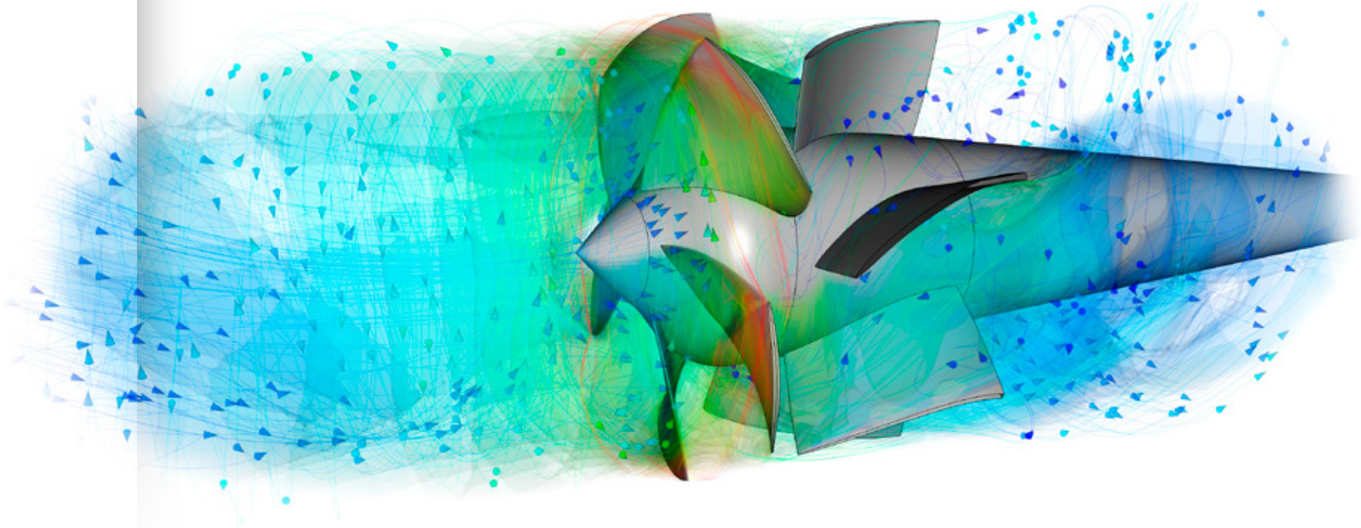
Significant reduction of **financial** costs



Tomáš Krátký

SIGMA GROUP a.s.

Our cooperation with IT4I has been very productive. The transition to "large" HPC has gradually become indispensable for the needs of pumping technology development. The technological intensity and our lack of experience with similar solutions, however, proved to be an almost insurmountable barrier. The experts at IT4Innovations have managed to contribute a complex solution comprising cluster configuration, running of computations, and custom-made solutions. Thanks to the fact that many of these experts have a high level of technical education and experience with joint projects with industrial partners, our communication was very smooth.



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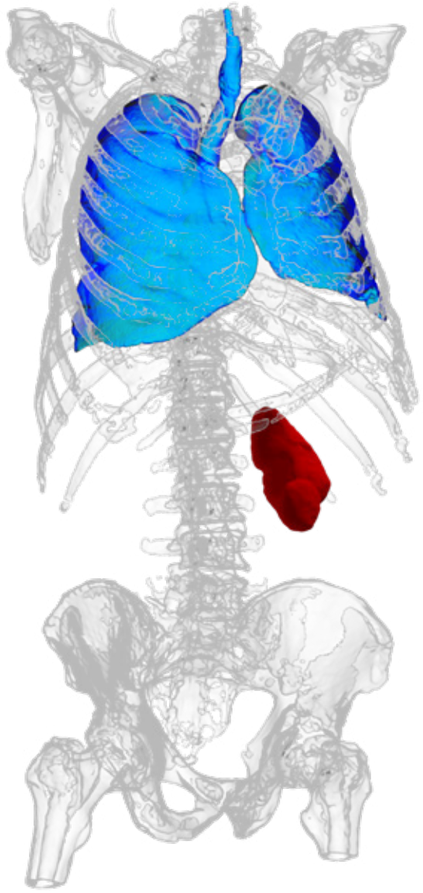
SUPERCOMPUTERS IN MEDICINE

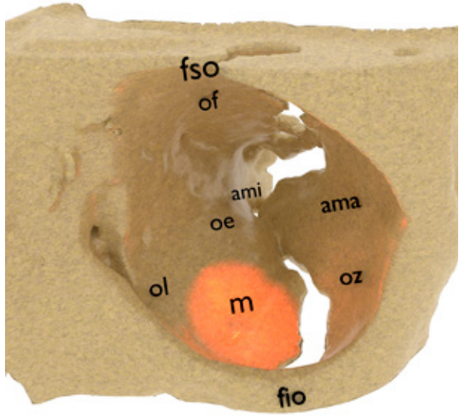
Partner: University Hospital Ostrava
Field: healthcare



Healthcare is one of the areas of human activity which generates a vast quantity of data, through the examination of patients. This volume is constantly increasing, which places more and more emphasis on their processing, storing, and securing. Examples of generally available diagnostic techniques generating enormous amounts of data are Computed Tomography (CT) and Magnetic Resonance (MR). Although the applied devices therein are equipped with software applications for creating virtual 3D models of organs based on CT or MR scans, this process is enormously time-consuming and labour-intensive, as it requires many inputs made by professional staff. The objective of the joint research work is not only to automate the process of creating 3D models from CT and MR scans but also to use it as a new source of further research.

One of the examples of using a 3D model for extracting normally unavailable information is precise measurements of orbital fracture size. This is one of the most important criteria when deciding whether a patient undergoes surgery or is given conservative treatment. However, this size can currently be obtained only approximately from CT scans and a simplified empirical approach.

Our researchers together with doctors from University Hospital Ostrava are developing a new method for precise orbital fracture size measurements using 3D models created from CT or MR scans. This new method, which not only uses image processing algorithms but also statistical methods, will allow more precise diagnostics in the case of orbital injuries.

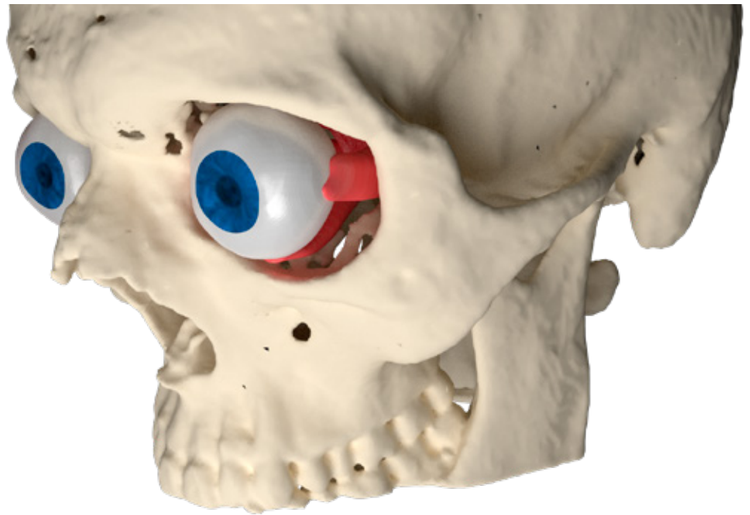


Orbital bone anatomy: fso – foramen supraorbitale, fio – foramen infraorbitale, ama – ala maior ossis sphenoidalis, ami – ala minor ossis sphenoidalis, oz – os zygomaticum, oe – os ethmoidale, ol – os lacrimale, m – maxilla. Maxilla is one of the most affected parts of the orbit.

Jan Štembírek

University Hospital Ostrava

Nowadays, measurements of orbital fracture defects by means of Computed Tomography (CT) examination are often imprecise and distorted for the irregular shape of the traumatically developed defect as well as the orbital floor. This information, however, can be crucial for a doctor to decide if a patient suffering these fractures undergoes a surgery or is given conservative treatment. Thanks to excellent cooperation with IT4Innovations, we are now developing a software application allowing us to make precise measurements of these defects as well as the orbital size based on CT examinations. This application might be a prospective tool for determining indicative criteria in orbital fracture therapy.



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DESIGN OF PASSENGER TRAIN SEATS

Partner	**BORCAD cz s.r.o.**
Field	mechanical engineering, transport industry

The cooperation between BORCAD cz s.r.o., one of the leading European producers of train seats, and IT4Innovations dates back to the year 2012. In this year, a joint team of researchers from IT4Innovations and designers from BORCAD cz s.r.o. was put together within a project supported by the Technology Agency of the Czech Republic (TACR) to develop a new generation of train seats for regional transport and long-distance travel. The essential requirement specified by the company was for the seats to fulfil strict safety criteria so they could be sold on the UK and Canadian markets. Safety is verified by crash tests. These tests are not only very expensive but also time-consuming because a physical prototype of the seat must be produced and sent to a certified laboratory for testing. If the test is unsuccessful the whole process must be repeated, which leads to an increase in the costs of new product development. Using virtual prototyping based on numerical modelling methods and simulations, it is possible to significantly reduce the risk of unsuccessful tests.

Within the testing process both integrity tests, when the tested seat must withstand an impact without being destroyed, and biometric screening tests, in which dummies are used as in the crash tests performed in the automotive industry, were performed. In the design of train seats, one major limitation is their weight, which must be as low as possible for competitiveness reasons. Furthermore, in order to fulfil the safety criteria defined by the UK standards, the seats must not only be sufficiently robust to withstand the crash tests, but also sufficiently flexible so that the biometric criteria for the dummy are fulfilled during its impact with the seat. Within the project implementation, the existing system of the seat prototype design and testing was modified so that all construction changes are first verified using a mathematical modelling method. When all criteria are fulfilled, only then is the physical prototype manufactured and sent to a laboratory for testing.

The first major achievement was the collaboration which led to certification of the seat Regio. The seat fulfils all of the strict dynamic requirements of the GM/RT2100 standard, and features a folding table, the inclusion of which increases the stringency of the certification process. Using parametric studies, the interval of the allowed seat pitch was significantly enlarged. Another research problem was the seat mounting to the chest of the wagon; a cantilever, which is subjected to significant bending and torsional stress during the dynamic testing. Within the research activities, several prototypes of the cantilever were designed. Two of them, including the Genio seat, were certified to the GM/RT2100 standard. Another important achievement was the design of safety modifications for the new seat Visio. The new technical solution ensures the upper part of the seat is minimally deformed by knees during impact. Based on intensive cooperation with applied scientists and designers, the certification of the seat was successful the first time it went through laboratory testing, without the need for modifying the prototype. It is also worth noting the successful cooperation during certification of the comfortable first class seat for the scenic railway in the heart of the Canadian Rocky Mountains. These seats fulfil the safety requirements given by the APTA PR-CS-S-016-99 standard, which is specific to North America.

The success of this cooperation was also recognised by the winning of the International HiPEAC (European Network of Excellence on High Performance and Embedded Architecture and Compilation) Technology Transfer Award. The cooperation between BORCAD cz s.r.o. and IT4Innovations is ongoing. The developed seat design system is still in use, with advantageous capability for the development of new seat types according to the specific requirements of new clients.

Tomáš Boruta

Sales & Marketing, BORCAD cz s.r.o.

Due to our mutual collaboration on particular problems, the level of knowledge and experience has been increasing throughout the company. I strongly believe that the results and benefits of our cooperation will soon be reflected in earning contracts in the UK market and wherever else passive safety in public transport plays an important role. The cooperation within the region has proven to be highly efficient, and for me personally it is still a source of interesting experience and delight for the many things which have been managed, which surpassed our original expectation.

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RENDERING AS AN EFFICIENT TOOL FOR UTILIZATION OF THE COMPUTING POWER OF SUPERCOMPUTERS

Partner **Blender Institute**
Field information technology

CC-BY-SA, Blender Institute, image from Open Movie Agent 327: Operation Barbershop – an example of the "wireframe" model and final visualization, based on comic series Agent327© by Martin Lodewijk

Visualization of computer-generated scenes where reaching a real-life appearance of displayed objects is required is a computationally highly intensive process. This can be achieved by rendering. At present, the most widely used renderers are those which can faithfully simulate the physical behaviour of light. Making use of such renderers, it is thus possible to achieve top quality results that are indistinguishable or nearly indistinguishable from real images.

In this field, IT4Innovations successfully cooperates with the Blender Institute, which is responsible for developing Blender. It is an open source 3D creation suite covering a wide portfolio of 3D computer graphics features ranging from creating a model, its animation to its final rendering. This is exactly where an opportunity to establish mutual collaboration has arisen. At IT4Innovations, the original Blender renderer, which could only be run on a computer workstation equipped with a graphic accelerator (GPU), was modified and further extended. Using the CyclesPhi module developed at IT4Innovations for rendering, it is possible to use the computing power of the entire supercomputer including its Intel Xeon Phi acceleration cards, which are fitted in about half of the compute nodes of the Salomon cluster.

With the use of the supercomputer, it is possible to achieve a reduction in the rendering time to a mere fraction of the original time. It is an example of an ideally scalable problem – this means that the ten, or hundred times higher the number of computational resources used, the ten, or hundred times shorter the computing time, respectively, etc. When creating the content, it is therefore possible to speed up the entire production process significantly. Within the collaboration with the Blender Institute, the Salomon supercomputer was used for rendering the following animated promo movies: Cosmos Laundromat: First Cycle, Agent 327: Operation Barbershop, and currently Spring as well.

The overall objective of the collaboration between IT4Innovations and the Blender Institute is to develop tools enabling remote rendering of 3D scenes and preparation of the Rendering as a Service package. As a result, rendering of complex scenes using the computing power of the supercomputing cluster will be made possible from any computer.

Francesco Siddi

Blender Institute

IT4I has been instrumental for the research and development process during the production of several Blender Open Movies. Having access to the Salomon cluster allowed for fast iterations during scene/performance debugging, and it also allowed the pursuit of high-end visuals, pushing rendering algorithms to the limits. The IT4I team has always supported our goals with great transparency and in the most professional way.

CC-BY-SA, Blender Institute, image from the Open Movie Cosmos Laundromat: First Cycle

CC-BY-SA, Blender Institute, image from the Open Movie Agent 327: Operation Barbershop, based on comic series Agent327© by Martin Lodewijk

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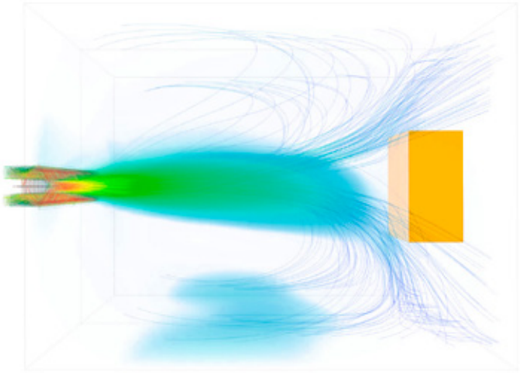
NUMERICAL SIMULATION OF ALUMINIUM PROFILES COOLING PROCESS

Partner: FERRAM STROJÍRNA s.r.o.
Field: mechanical engineering



The aluminium profile cooling process must be fully under the control of water quench operators. In the production process, an aluminium profile leaves the extrusion die at a temperature of approximately 500–550 °C, which needs to be reduced to the required temperature of 200–250 °C in a relatively short time of 15–30 sec. This can be achieved by treating the profile surface with water-air spray cooling in the water quench using special nozzles.

FERRAM STROJÍRNA s.r.o. is one of the world's leading producers of cooling equipment for extruded aluminium profiles. This company has developed a revolutionary shape of jets, which allow a large volume of water and air to be accelerated at low pressure so as to achieve the desired effect of heat being conducted away from the profile surface. The specially designed nozzle forms droplets of water, which are subsequently mixed with air. These droplets are then carried away by air flow and spray the profile surface, conducting the heat away, thus cooling the profile. The correct setting of the Water Quench varies according to the shape of each individual profile. This setting is largely dependent on the experience of operators, which makes repeatability and precision of this process harder. In new profiles with no preceding setting, this leads to a high scrap factor as a result of using the trial and error approach.

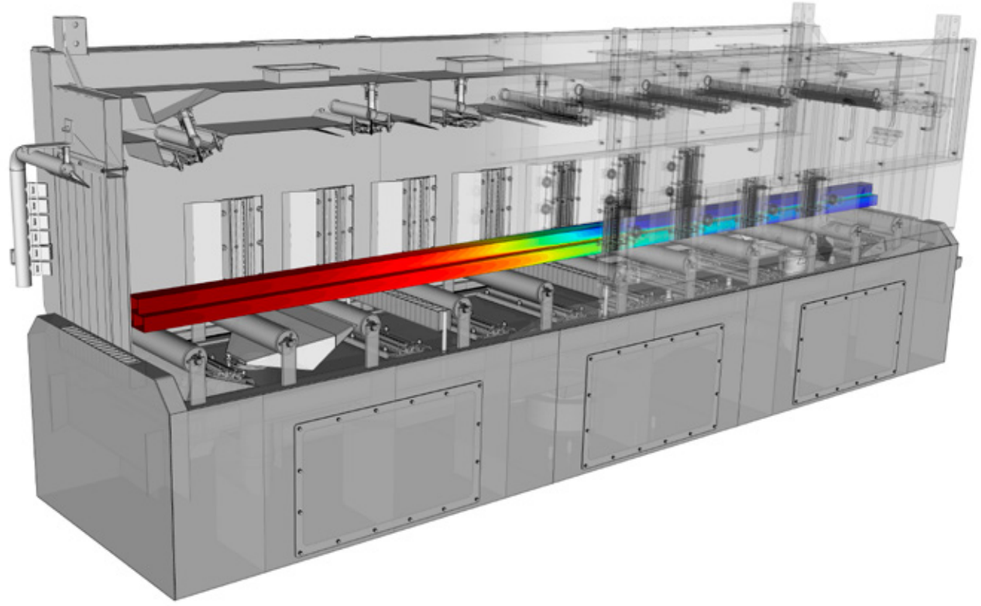
Within the European H2020 CloudiFacturing project, IT4Innovations and FERRAM STROJÍRNA s.r.o. cooperate in developing a numerical fluid flow model to simulate the aluminium profiles cooling process. Given the need to include all important physical processes associated with the aluminium profiles cooling process, a numerical model of the whole Water Quench, containing seven separate sections each equipped with four rows of nozzles, needs therefore to be developed. In addition, each nozzle must be modelled down to the slightest detail, which leads to hundreds of millions of compute cells in the resulting numerical model. Such a complex model cannot be solved using generally available workstations in a reasonable time. Its solution would take several weeks and therefore using supercomputers seems an ideal option.

In the future, the newly developed and experimentally verified method based on CFD simulations will be used by FERRAM STROJÍRNA s.r.o. in developing a new generation of nozzles allowing brand new profiles to also be produced, which otherwise could not currently be cooled down to the required temperatures using the existing cooling equipment.

Ondřej Tůma

Managing Director
FERRAM STROJÍRNA s.r.o.

In our field, it is no simple task to find a partner who is not only a top expert in a given field but also able to take initiative in finding innovative solutions. It is only in more challenging situations when cooperation with real professionals is genuinely appreciated. IT4Innovations has certainly been the right choice, making us happy to turn to their experts in the future.



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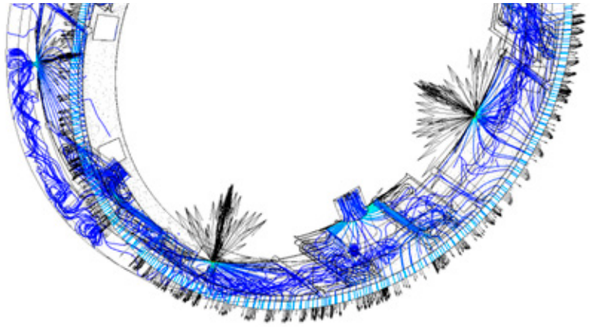
STUDY OF THE DYNAMICAL PROPERTIES OF SQUEEZE FILM DAMPERS

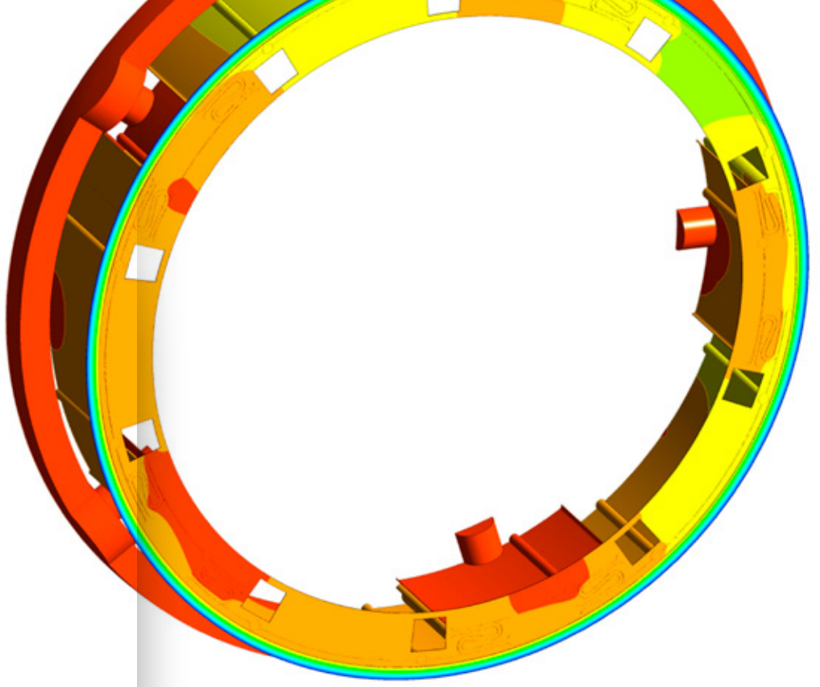
Partner	Doosan Škoda Power s.r.o.
Field	mechanical engineering, energy industry



IT4Innovations cooperates with Doosan Škoda Power s.r.o., which is a leading producer and supplier of highly efficient steam turbines (with a capacity of 10 MW to 1200 MW), technological equipment, and 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 transverse oscillation 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 proven 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.

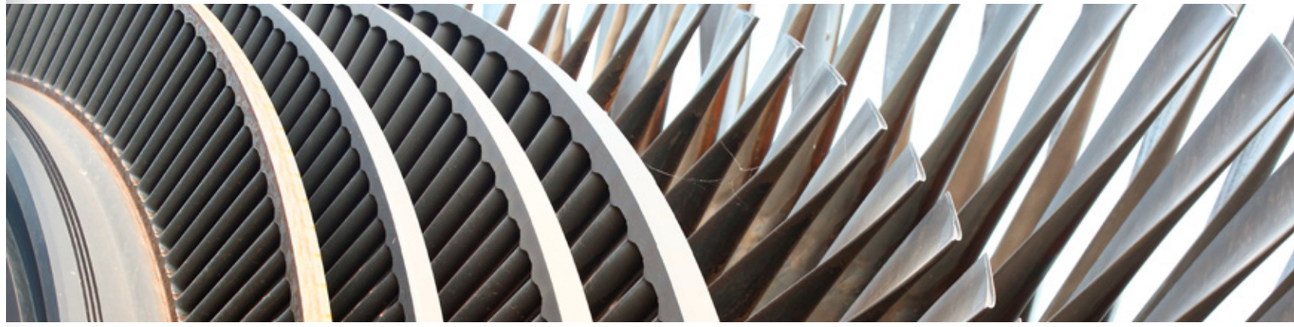


PARTNER´S NOTE

Václav Polreich

Head of Measurements and Diagnostics
Doosan Škoda Power s.r.o.

The mutual cooperation was 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, and thus contributing to more flexible and smooth running of these machines. The cooperation with the IT4I researchers was very productive. They possess 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.



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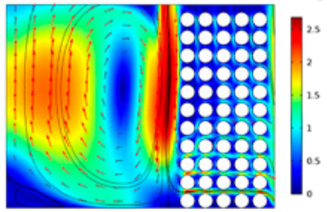
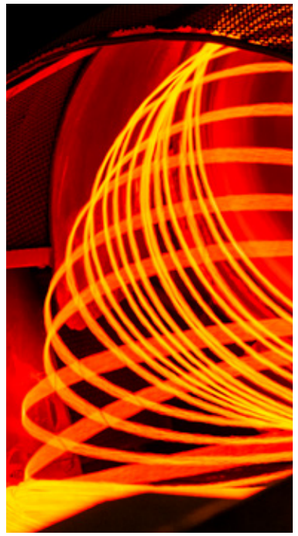
DEVELOPMENT OF NUMERICAL MODELS IN THE METALLURGICAL INDUSTRY

Partner	ITA spol. s r.o.
Field	mechanical engineering



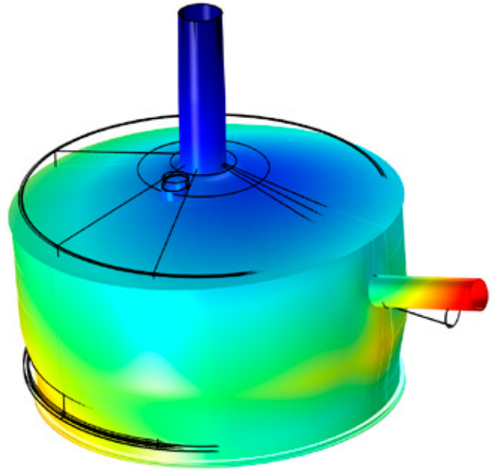


The researchers at IT4Innovations have a long-term cooperation with the ITA spol. s r.o. company based in Ostrava, the Czech Republic. This company was established in 1991 and has since then been involved in solving technical problems in the metallurgical industry in the Moravian-Silesian region and elsewhere. ITA spol. s r.o. is engaged in advanced hot and cold rolling technologies, rolling mills control system optimization, computer modelling of metallurgical processes, and solving technical problems and technological innovations in hot and cold rolling mills.

The cooperation with industrial partner ITA spol. s r.o. includes development of numerical models, execution of computer simulations on powerful workstations or supercomputers, and engineering evaluation of the results achieved. This cooperation has lately been performed within research projects supported by the Moravian-Silesian region.

An example of such common research activities is a project entitled Computer simulation of rollers cooling during the rolling process with the aim to optimize the quality of the rolled product and service life of rollers. Within the project, a numerical model was developed along with performing computer simulations of stress, strain, and thermal fields, and on this basis optimization of the roller cooling process was executed. Consequently, improvement of technical and economical parameters of production was achieved as a result of reducing the consumption of cooling water, prolonging the service life of rollers, and enhancing the quality of the rolled product.

Another joint activity included project computer modelling of thermal fields in wire and strip coils. In order to maintain the desired mechanical properties of steel wires and strips, the rolling process must be followed immediately by their controlled cooling, where the temperature is kept within a specified range. The control systems for optimal cooling take advantage of temperature prediction, and therefore an efficient computer model to calculate the thermal field in a coil was developed within the project implementation.



Daniel Hajduk

Executive Manager
ITA spol. s.r.o.

Our cooperation is unique for the fact that the experts at IT4Innovations have knowledge of the engineering background of the solved problems, which they then apply in computer model development. Moreover, they know and are able to use fast and efficient algorithms to solve these problems using computer workstations as well as supercomputers.

In the upcoming period, we would like to cooperate with IT4Innovations in joint research focused on developing multiphysical models of technical problems, which we aim to solve using our own software products. For the complexity of these models, however, we are not able to develop them on our own.

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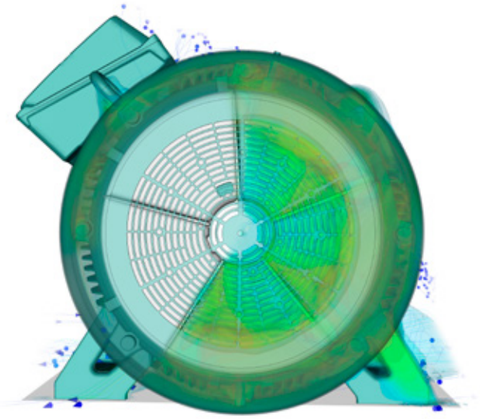
FAN SECTION OPTIMIZATION IN ASYNCHRONOUS ELECTRIC MOTORS

Partner	**Siemens Electric Machines s.r.o., Frenštát**
Field	energy industry, mechanical engineering



In cooperation with experts from the Siemens company, we are pursuing development of optimal fan section design in order to improve the cooling efficiency of asynchronous electric motors. Siemens Electric Machines s.r.o., Frenštát is one of the leading producers of low-voltage asynchronous electric motors. Their primary customers are producers of pumps, compressors, and air-conditioning equipment. One of the priorities of the Siemens company includes the production of electric motors with highly efficient cooling systems, allowing smooth operation of these machines even under extreme conditions.

If the design of the active fan section is to ensure efficient cooling of the electric motor, it is important to secure a supply of the highest possible volume of air, which is further distributed over the maximum possible surface of the electric motor frame in order to secure sufficient exhaust ventilation of heat generated by electro-magnetic phenomena. The optimized design of the fan section shall prevent its construction from negatively affecting the running of the electric motor, which would result in an increase in mechanical losses and excessive noise generation.

In order to find the optimal design meeting the above-mentioned parameters, tens of CFD simulations shall be performed. Using the HPC infrastructure available at IT4I in combination with the application of an open source software solution, CFD simulations can be performed for the whole electric motor with no shape simplifications required. Taking this approach, laboratory measurements can be fully replaced by a virtual model, which would in turn accelerate the process of designing the fan section as well as allowing the impact of each individual modification on its functionality to be assessed with no need for producing the physical prototype.

Using the IT4I infrastructure in synergy with the available know-how in CFD simulation areas, several experimentally comparable steady state and fully transient CFD simulations can be performed on a full model of the electric motor without any geometrical simplifications within two hours and two days, respectively. Simulations of one design using a common workstation, as opposed to using a state-of-the-art HPC infrastructure, takes days for steady state CFD simulations and months for a single, time-dependent CFD simulation, which makes it impossible for the design to be developed using virtual prototyping.

WORK STATION

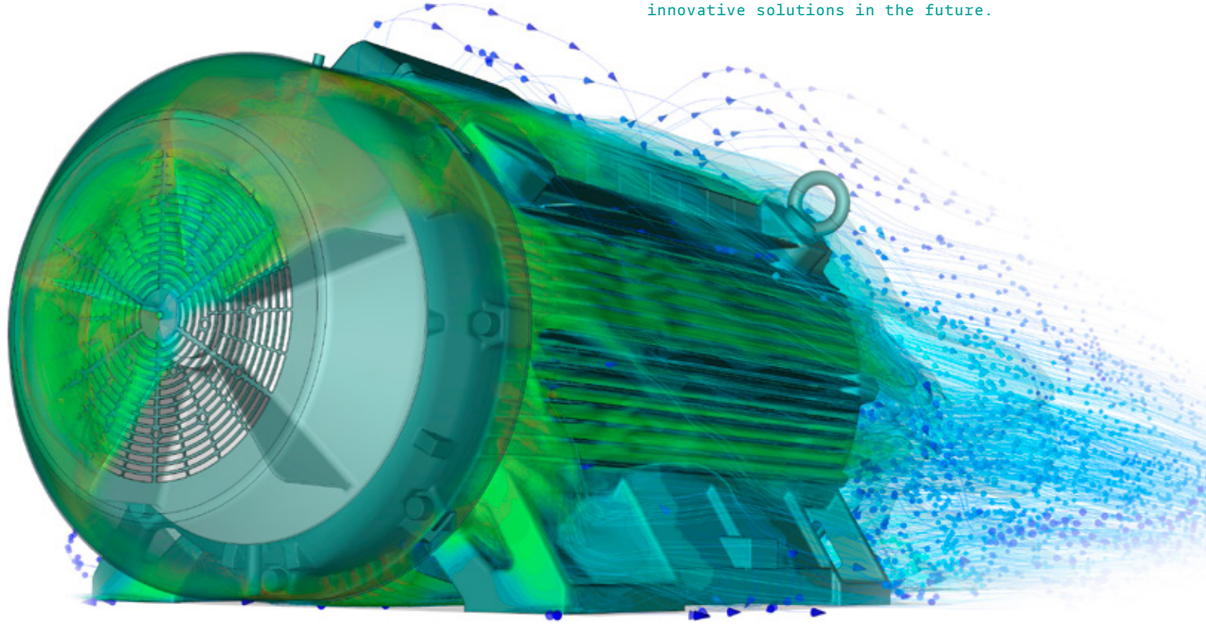
HPC CLUSTER

Considerable time saving
when using HPC as opposed to
a standard workstation for design

Igor Majer

Head of Research and Development Hub Ostrava
Siemens s.r.o.

Although our cooperation with IT4Innovations National Supercomputing Center is in its early stages, we are fully aware of its potential for innovation and research projects areas. Nowadays, we can often catch buzzwords such as Industry 4.0, digitalization, or digital twins. This particular research project successfully demonstrates that many interesting digitalization projects have been implemented in Siemens.
I am firmly convinced that these joint activities not only offer great potential for increasing the competitiveness of our products but also the prospects for many innovative solutions in the future.



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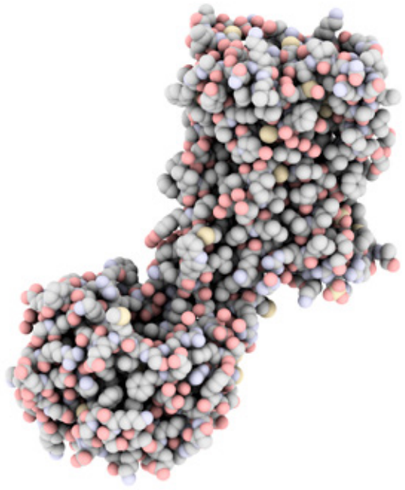
MACHINE LEARNING FOR DRUG DISCOVERY

Partner **Janssen Pharmaceuticals**

Field information technology, pharmaceutical industry



Machine learning applications are becoming increasingly used in various areas of human activity such as the energy industry, industrial automation, robotics, the automotive industry, and biomedicine. At an industrial level, these applications usually include a series of mutually interconnected data processing steps.

Within the framework of the European ExCAPE project funded by the Horizon 2020 programme, we cooperate with pharmaceutical companies in the field of drug discovery using supercomputers and machine learning methods. The opportunity to exactly predict the activity of chemical compounds enormously reduces the costs and time required for this process, and has a significant impact on innovation in therapeutic processes and increasing the possible uses of medication.

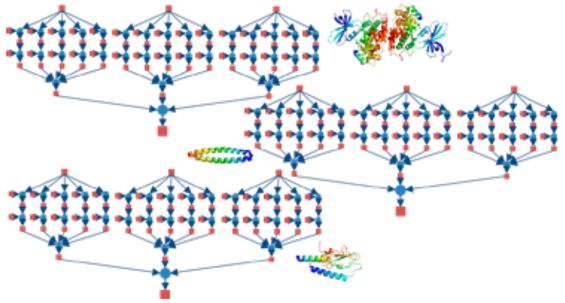
For this purpose, a number of tools allowing us to face this challenge have been developed. The contribution of IT4Innovations is the open source software HyperLoom, which allows dependent computational tasks to be efficiently distributed in distributed environments.

HyperLoom users can easily define dependences between computational tasks and create a pipeline, which can then be executed on an HPC system. This software also allows users to execute pipelines containing a wide range of task types, from basic built-in tasks and user-defined tasks to tasks wrapping third-party applications including their combinations.

HyperLoom was designed to have minimal task planning and running overheads, and to efficiently deal with the varying execution times of different tasks. The software core is implemented in the C++ programming language and is able to dynamically orchestrate tasks over available computational resources with respect to user-defined task requirements. The core of HyperLoom is composed of a server and several worker components. The server component is responsible for planning and running tasks on worker components, which run on compute nodes. Pipelines are then defined and sent to the server via a Python interface.

Performance tests have proved that HyperLoom allows execution of pipelines containing hundreds of thousands of interconnected tasks with unknown execution times on tens to hundreds of compute nodes. In addition, this universal tool is also applicable in other industrial sectors.

HyperLoom is an open source product available at IT4Innovations GitLab including the relevant documentation and use cases under the BSD3 licence.



Vladimir Chupakhin

Janssen Pharmaceuticals

Pharma companies have collected a significant amount of protein-ligand interactions forming the so-called chemogenomics matrix: interactions between compounds and proteins. However, this matrix is very sparse with less than 1% of this matrix being filled. Predictive modelling can help fill this matrix using a classification or regression model. Predictions in turn are used to speed-up the drug design and development process, which can help cut costs as well as reduce animal use. While machine learning is widely used in every step of the drug design and discovery process, it is still a hurdle to use it on big data, taking into account all of the modelling steps needed: hyperparameter search, model and predictions storage, etc. Together with IT4Innovations, we try to overcome these challenges within the ExCAPE project.

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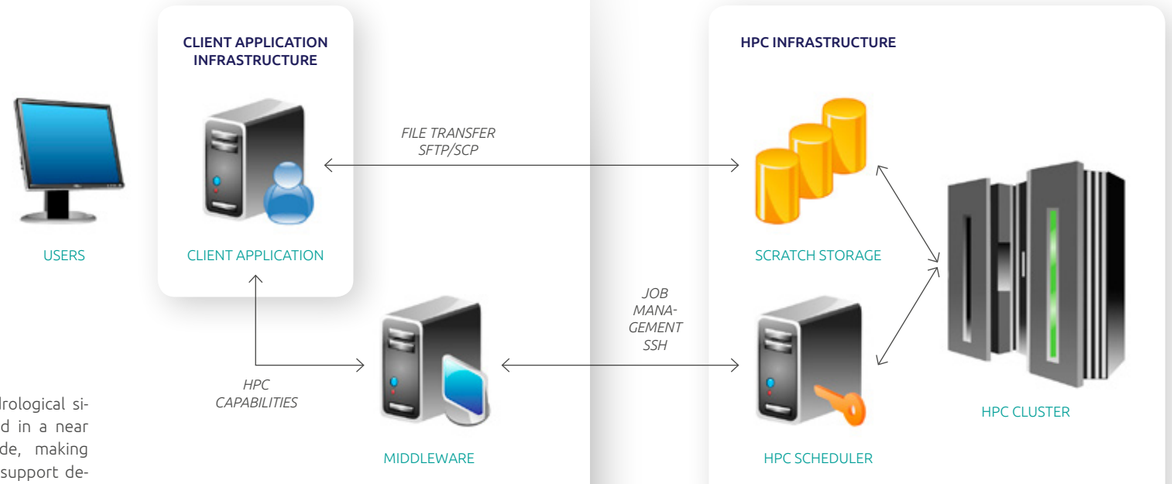
“HPC AS A SERVICE” FOR HYDROLOGICAL MODELLING

Partner	DHI
Field	information technology, water management, environment



Risks and uncertainties have become the key aspects of the vast majority of decision-making processes. The qualitative assessment of risk is usually based on perception, opinions, judgments, and public or political consensus (or their combination), while the quantitative assessment of risk is based on the results of modelling methods. To perform disaster risk analysis, modelling techniques using on-line monitoring data are often required. In this context, the ratio between the run time and real time of the modelling cycle is an important aspect. Powerful personal computers are not often able to run models at a sufficiently fine scale fast enough to obtain relevant results in the required short time. These results are needed for prognosis and forecasting but mainly for the reaction phase itself.

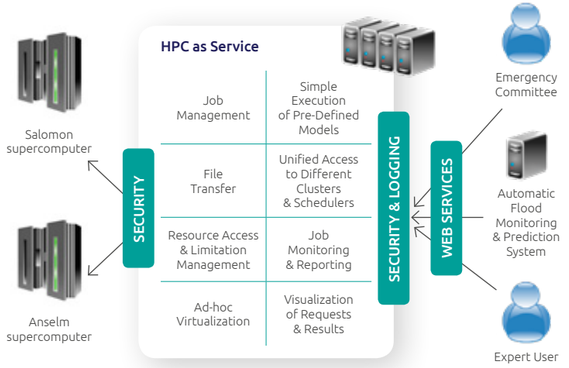
“HPC as a Service” in hydrological modelling allows hydrological models to be remotely operated on HPC clusters. Using HPC, results of hydrological simulations can be obtained in a near real-time processing mode, making these results available to support decision making in emergency situations as well as providing possible preventative measures for reducing the risks and extent of such emergency situations in the future. Moreover, parallelization of a hydrological model and its remote running using HPC also allow users to increase the accuracy and precision of results by increasing the resolution of meshes whilst maintaining a manageable runtime.

For remote running of hydrological modelling processes on an HPC infrastructure and automated monitoring and prediction of floods, we created an application interface originally known as “HPC as a Service” in collaboration with the DHI company operating in the fields of water management and the environment worldwide. This interface integrates an approach to various HPC systems via an object-oriented client-server interface and standard web services. Furthermore, it ensures the availability of desired support functions, such as task management, resource monitoring, messaging, user verification, data transfer, encrypting, and various notification mechanisms. The new generation of the developed HPC as a Service application interface is known as HEAppE (High-End Application Execution, http://heappe.eu). At present, HEAppE is successfully used in several public and commercial projects (not involving only on hydrological modelling), where remote access to an HPC infrastructure is required.

Johan Nicolai Hartnack

DHI

HPC as a Service significantly lowers the entry barrier for users who are interested in using massively parallel computers for efficient running of their simulations. Taking advantage of this service, small and medium-sized enterprises may use this technology with no initial investment in hardware.



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PROCESSING AND STORING DATA FOR THE EUROPEAN SPACE AGENCY

Partner **ESA**

Field information technology, Earth sciences

Joint research in this field is carried out within the Urban Thematic Exploitation Platform project of the European Space Agency in collaboration with the German Aerospace Center (Deutsches Zentrum für Luft- und Raumfahrt, DLR), GISAT and others.

The expanding operational capability to acquire a huge amount volume of data from space 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 program was to develop and implement a number of thematically oriented platforms, virtual environments facilitating the search for data acquired by Earth observation. These platforms provide user communities not only with access to the mass data archives of EO missions but also with the information and communication technology needed for their effective processing, analysis, and visualization. Currently, the TEP program includes the Coastal, Forestry, Geohazards, Hydrology, Polar (polar areas), Food Security (food cultivation sustainability), and Urban (population) platforms. IT4Innovations is actively involved in the last one mentioned – the Urban Thematic Exploitation Platform (Urban TEP).

The general TEP idea follows the principle of bringing users to the data and analytics tools. 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 include, for example, generation of cloud-free mosaics of the Earth's surface to provide a consistent view of the built environment, tracing global urbanization, regional land-use dynamics, and the deployment of processing functionalities for the derivation of orthomosaics and digital surface models from drone data.

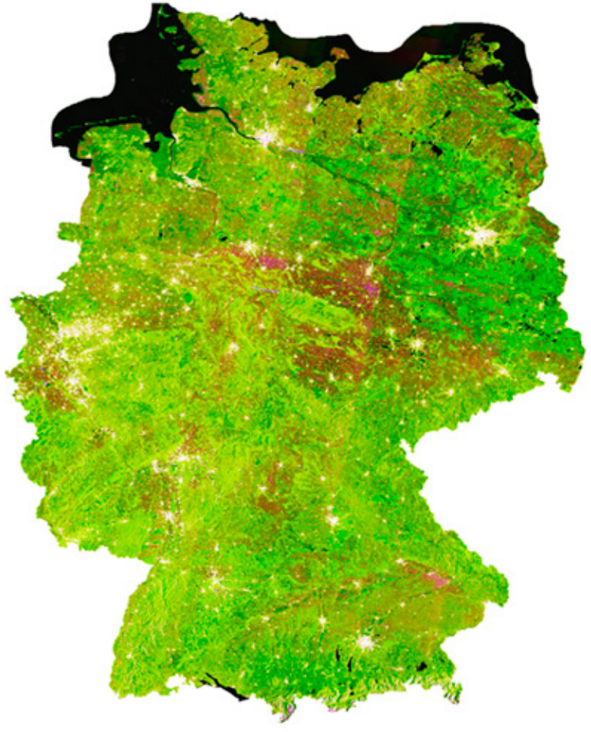
The Urban TEP is operated by an international consortium of five partners, including the German Aerospace Center (Germany) as the lead and Brockmann Consult GmbH (Germany), Terradue Srl (Italy), and IT4Innovations National Supercomputing Center and Gisat s.r.o. (Czech Republic). DLR and Brockmann Consult 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 joint analysis and visualization of all data layers available at the platform.

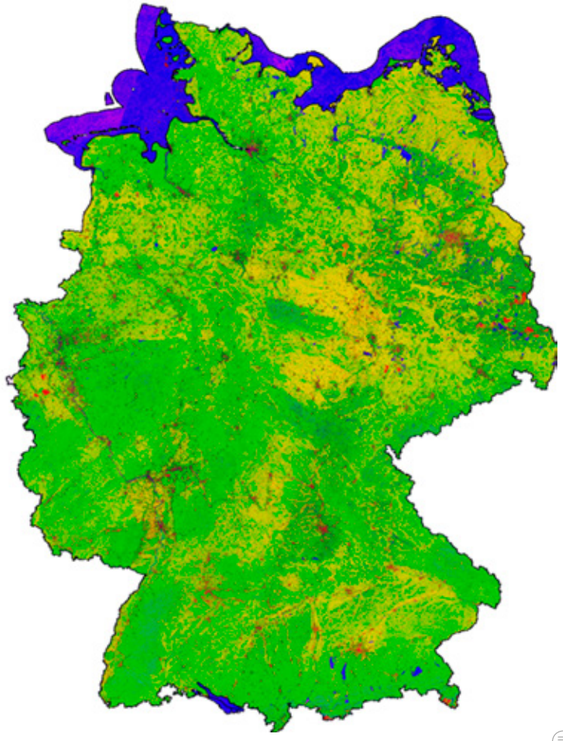
In the next phase, the Urban TEP activities will focus on a systematic enhancement and streamlining of the platform capabilities and product/service functionalities to meet the requirements of a fully operational and sustainable platform.

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

Interest in the use of the Urban TEP platform

As of the end of the Urban TEP pre-operations phase in June 2018, more than 300 institutions from more than 40 countries have expressed interest in the products, services, and system access, with 40% of the users coming from the scientific community, 30% from public institutions, 20% from non-profit/ non-governmental organizations, and 10% from the commercial sector.





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PRECISE EVALUATION OF VERTICAL MOVEMENTS USING SYNTHETIC APERTURE RADAR SATELLITES

Partner	Gisat s.r.o.
Field	geology, geodesy

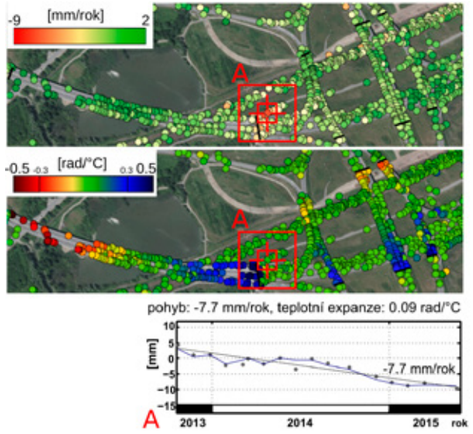
In cooperation with professional companies within a TACR (Technology Agency of the Czech Republic) project, we are involved in the development and application of algorithms for Interferometric Synthetic Aperture Radar (InSAR), which enables identification of primarily vertical movement of built structures (buildings, bridges, etc.) with an accuracy often exceeding 1 mm/year. The sensitivity of synthetic aperture radar (SAR) satellites to movement opens the door to their potential use for identification of terrain changes, such as synclinal valley development in undermined areas, and detection of landslides.

Data generated by SAR satellites have already been available since the 1990s (Europe Sensing Satellites - ERS, resolution of 25x5 m, imaging every 35 days). The latest SAR satellites enable very high resolution (Cosmo or TerraSAR-X - standard resolution of 3x1 m, revisit cycle of a few days; Sentinel-1 – resolution of 4x20 m, revisit cycle of 6 days), which is an advantage in continual scanning and open data access. For accurate analysis, primarily the Persistent Scatterers method is used to process time series of at least 30 images. With the increasing number of images, not only the accuracy of results but also storage and computational resource requirements are increased.

Complex processing of a huge amount of radar image data using an HPC infrastructure is a question of several minutes, while using a standard workstation these computations take several days. The IT4Innovations infrastructure provides computational resources enabling independent running of computations over various data sets or fields of interest. As each compute node is exclusively allocated, the collaborators can thus perform computations with a fast response and a graphical user interface without being limited by the overall utilization of the infrastructure.

For performance of experiments, the commercial SARPROZ software and developed in-house codes have been used. Building on the experience gained from the previous cooperation, we have developed our own solution, namely the IT4SI application, which allows efficient use of HPC for InSAR processing of data generated by the Sentinel-1 satellite. This solution has been partially implemented into the Floreon+ platform for support of crisis management in the Czech Republic. The objective is to automate the demanding approach to processing so that the technology is applicable for experts with no deep knowledge of InSAR.

The project of the Technology Agency of the Czech Republic named "Monitoring of undesired movements and deformation of transport infrastructure using radar interferometry" was evaluated as the best one in its category for the 2018 TACR award.



Jan Kolomazník

Technical and project manager
GISAT s.r.o.

Cooperation with IT4I within the project focused on detection of undesired transport infrastructure deformations via satellite data has been very productive for us. Processing of long time series of satellite images using radar interferometry is computationally intensive, and its deployment on HPC infrastructure has enabled us to significantly streamline and speed up the computing process. Having no previous experience with deploying this technology, using the cloud services of IT4Innovations National Supercomputing Center, we have immensely appreciated the support provided by the IT4I experts who assisted us in cluster configuration and in design of the computing solution as well as of the processing scripts. Therefore, we look forward to building on our latest cooperation in the future.

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STOCK INVENTORY CONTROL OPTIMIZATION BASED ON SALES FORECASTING

Partner	**K2 atmitec s.r.o.**
Field	information technology, logistics

Nowadays, it is necessary for production companies to pay attention to efficient use of storage premises. It is far too complex for people to monitor all stored products in real time, and that is exactly where information technology using state-of-the-art statistical methods comes into play.

K2 atmitec s.r.o. is the developer and supplier of the K2 information system for assisting in control and optimization of business processes via a complex system based on business data analysis. One of the incremental innovations here is the integration of a stock inventory control system, which is based on a module for sales forecasting developed within an established collaboration with IT4Innovations. This module allows the movement of stored goods in the previous period to be analysed, future sales to be forecasted using statistical methods for time series analysis, and excessive stock inventory to be eliminated. As total sales of several companies were analysed during the module development, a huge amount of data was processed, which led to building and comparing numerous statistical models. To verify the effectiveness of the developed module, an enormous number of computationally intensive simulations of stock development had to be performed using the supercomputer. Within our next collaboration, the supercomputer was used to search for the optimal parameters of models for stock inventory optimization.

Regarding the sales forecasting module, the IT4Innovations team deals with data such as order point, safety stock inventory, and economic order quantity set from sales forecasts based on historical data, where the service level can be adjusted by the user. These predictions are based on statistical methods for time series analysis. Various data types are treated: raw data, purified data, filtered data, and data with daily, weekly, and monthly aggregation. For all combinations, several models have been built: linear, quadratic, cubic, and ARIMA. Using the MASE (mean absolute scaled error) comparative criterion, each model is automatically compared, and the best one of them is then recommended for further calculations.

Stock inventory control optimization based on sales forecasting allows the decision time to be reduced, warehouse operations to be facilitated, and costs to be reduced as a result of stock inventory optimization.

Petr Schaffartzik

K2 atmitec s.r.o.

Together with the development of information technology, companies expect their business information systems to make a more and more significant contribution to automation of processes. One of the areas where companies are fully dependent on human skills and knowledge is stock inventory control. We aimed to provide our clients with tools which would make the purchase process even more automated. We were also aware of the fact that we were missing the necessary experience and know-how to manage this on our own. Therefore, we decided to establish cooperation with IT4Innovations, where we could acquire the needed know-how, assistance with development, and testing in selected companies. In the K2 information system, our clients are offered unique functionality, which they would otherwise have to solve by integration of another complex system.

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PLATFORM FOR PARALLEL PROCESSING OF DNA SEQUENCES

Partner **MOLDIMED**

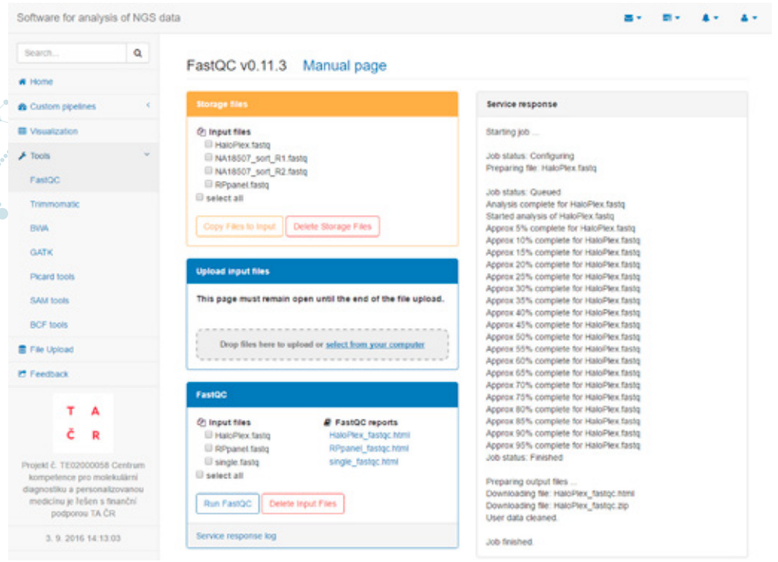
Field bioinformatics

Joint research in this field is carried out within the Center of Competence for Molecular Diagnostics and Personalized Medicine project under the Technology Agency of the Czech Republic, where we jointly collaborate with CEITEC, University Hospital Brno, University Hospital Olomouc, GENERI BIOTECH s.r.o., IntellMed, s.r.o., Palacký University Olomouc, and the Institute of Molecular Genetics of the Czech Academy of Sciences.

Massively parallel sequencing (MPS) approaches play a key role in clinically focused research and DNA molecular pathology diagnostics. The concept of personalized medicine thus replaces classical approaches, which are often methodically time-consuming in terms of covering long DNA sequences. Whole Exome Sequencing (WES), amplicon sequencing of long PCR products, and sequencing of gene panels associated with specific diseases are all methods currently used to verify genetic risk factors. MPS methods such as WES, in particular, generate a huge amount of data, which needs to be further processed.

Therefore, a platform for processing next-generation sequencing (NGS) of data for detecting hereditary and somatic DNA variants was developed within the Center of Competence for Molecular Diagnostics and Personalized Medicine project under the Technology Agency of the Czech Republic. The platform is applicable for genomic/exome and panel DNA sequencing projects.

The main objective of the platform is to provide researchers focused on clinical MPS data with easy and intuitive access to the HPC infrastructure via a specialized web interface. The platform contains its own annotation tool developed by the MOLDIMED centre and a number of freely available bioinformatics tools. The platform is currently being operated in two independent instances using the HPC infrastructure of IT4Innovations and MOLDIMED centres.



Web platform for MPS data processing

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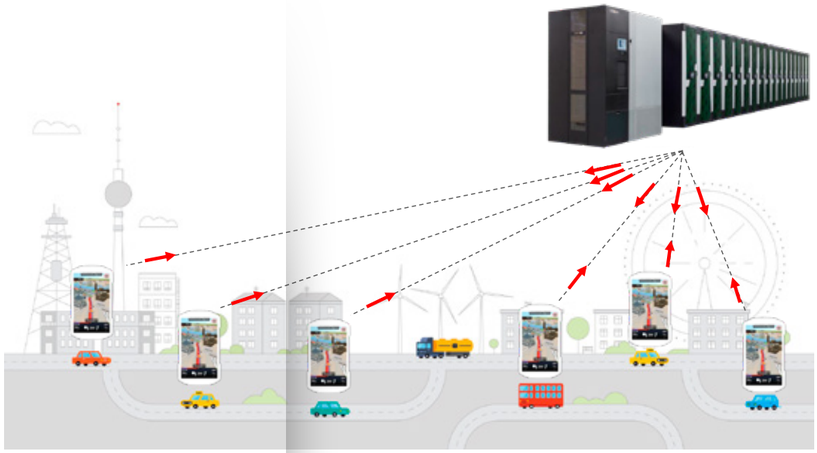
WHAT HAPPENS IF ... ANALYSES FOR SMART CITIES IN COOPERATION WITH SYGIC, THE GPS NAVIGATION PROVIDER

Partner	**Sygic, a.s.**
Field	information technology, Smart City



The Smart City is a concept aiming to increase the quality of many aspects of our life in modern cities with respect to reduced energy consumption. These include, for example, traffic optimization, efficient control of air-conditioning and heating in buildings, easier access to public services, etc. In the field of traffic management, for instance, cities need to know what would happen if a road was closed for bridge reconstruction work, the road narrows, or if there is overload of the road network because of a mass sports event. Such information is valuable for authorities responsible for transport infrastructure operation in managing potential crisis situations, and in efficient planning of road network repairs at an appropriate time so as to minimize their impact on traffic flow.

In cooperation with the navigation company Sygic, a.s., we are focused on the aspect of traffic optimization in cities in the form of developing specific services based on advanced data analyses and simulations as well as an expert, self-adaptive navigation system combining client and server-side routing. This system uses historical data, up-to-date traffic flow monitoring, and graph theory based methods for determining the potentially busiest sections within the transport network. Furthermore, the system is extended with integration of population mobility data. For macromodelling within the system, we use our own implementation of a betweenness centrality algorithm, which is being further improved through conducting research and development. Application of this algorithm to large graphs, which represent a large number of road segments, is very computationally intensive and therefore we use the supercomputing infrastructure so as to provide up-to-date information to users as fast as possible.

Efficient provision of such created services is secured using the technologies developed within the ANTAREX project under the EU H2020 programme. The main objective of ANTAREX is to provide methods for mapping, real-time administration, and autotuning for HPC systems with respect to efficient energy consumption. In order to do so, tools based on LARA, a specific domain-oriented language for heterogeneous systems, have been developed. In combination with autotuning, it is thus possible to efficiently apply the principles of parallelization, scalability, and dynamic self-adaptability to fully utilize the power of an HPC system.

The results generated within this cooperation have been applied within the ANTAREX project, published in a number of articles, and last but not least presented to the general public at conferences including SC 16 (the International Conference for High Performance Computing, Networking, Storage and Analysis) held in Salt Lake City as well as at Transportation Research Arena 2018 in Vienna.

http://www.antarex-project.eu

Radim Cmar

Sygic, a.s.

Our cooperation with IT4Innovations and taking advantage of their experience and resources in the field of supercomputing and traffic modelling extend our skills and provide large-scale transport analysis for cities in near real time, which makes our product very competitive on the current global market.

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ANALYSIS OF CAUSES AND PREDICTION OF PROBLEMS IN 4G AND 5G NETWORKS

Partner	T-Mobile Czech Republic a.s. Deutsche Telekom-IT Competence & Delivery Centre Prague – CDCP
Field	telecommunications

In cooperation with the competence centre for Deutsche Telekom networks development operated by T-Mobile Czech Republic a.s., we are involved in performing analysis of data generated from the backbone network of the mobile operator in order to increase reliability and reduce cost in maintaining new technologies ensuring 4G and 5G mobile networks operation.

High reliability of telecommunication networks is ensured by sub-analyses performed for each technology or network unit. However, a number of technical problems in networks are caused by a combination of their various parts or technologies. Therefore, it is difficult to identify the causes of these problems using the existing approaches and methods. Moreover, identification of the root cause is also time-consuming. The objective of the collaboration is to find the key data sources, gather information about technical problems in one place, and identify performance indicators, which can be used to increase reliability and prevent problems in the network. The results will be verified in a testing environment, which must be compatible with the production environment available to the industrial partner.

The joint research aims to analyse the data obtained from the backbone network of the mobile operator, in particular from those parts ensuring network rules and billing. One of the main tasks is to work out the procedures followed by analyses both leading to identification of problems in the implemented voice technology for the Voice over LTE (VoLTE) service, which stands for Voice over Long Term Evolution. VoLTE supersedes older voice technologies in mobile networks against which it introduces an enormous conceptual difference. The various alternative implementations of the technology cause problems with mutual cooperation of the network entities.

Our analysis is focused on basic indicators in the network, such as volume of disconnected calls or reported errors of the used protocol. Based on these errors, the key performance indicators are proposed. Regarding the nature and volume of the data analysed, specific tools for big data analyses need to be applied. The current results indicate that most of the problems with the VoLTE technology are associated with particular mobile network terminal equipment and cells, which do not appropriately cooperate. This is caused by unanchored specification of VoLTE and the large number of suppliers of mobile devices operating within a single network. These problematic devices in particular mobile cells have been detected by applying the developed anomaly detection algorithm, which uses a selected key indicator. An important property of the performed analyses is the opportunity to geographically locate all events using various data layers, which significantly simplifies their solution on the side of the mobile operator.

Due to the dispersion of polygons representing the model of mobile network coverage, the very display of relevant network layers for analytical purposes presents a significant technological challenge, despite the progress in public availability of thematic base maps. Based on the past experience, we are preparing data files structures over a longer period to allow time series analyses using the proposed indicators. Pre-processed data sets and processing procedures enable us to use reliable statistical methods such as seasonal and trend breakdown to find anomalies that may appear quite irregularly.

Radim Kalfus

Telco Development team
Competence & Delivery Centre Prague – CDCP
T-Mobile Czech Republic a.s.

For implementation of this solution, we use not only the HPC infrastructure but also the experience of experts in data arrangement conception and design, parallelization of computations, and algorithm optimization. The parameters obtained from HPC simulation will serve as input for a solution, which shall not require HPC power thereafter. Future integration using machine learning offers us a unique opportunity to automatically detect and classify anomalies in the network as well as to increase the availability of services to end customers by means of timely reconfiguration.

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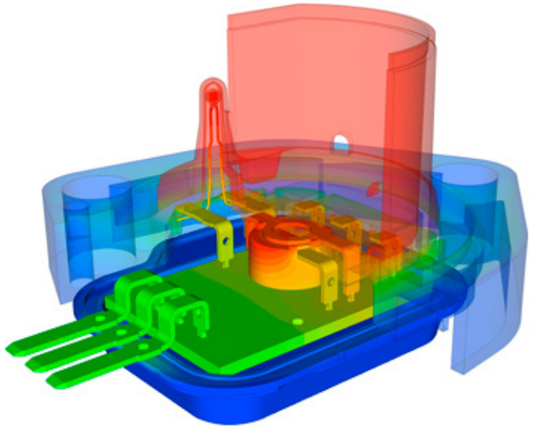
RESPONSE TIME OPTIMIZATION

Partner	Continental Automotive Czech Republic s.r.o
Field	automotive

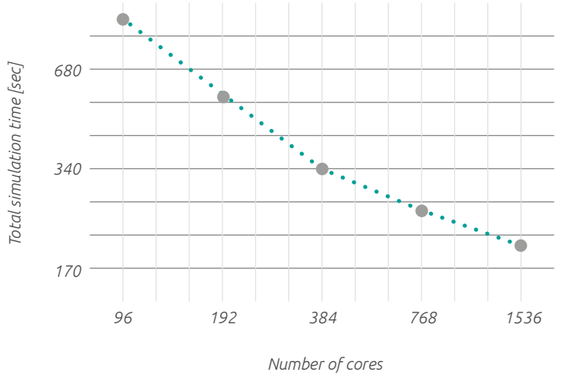


Together with the research and development staff of Continental Automotive Czech Republic s.r.o., a tool for speeding up the design of thermal sensors and their optimization was developed.

In the thermal sensors design, it is necessary to ensure their fast response to the fullest possible extent of the operational parameters such as changeable ambient temperature given by the climate change or rapid change in temperature of the measured operating fluids.

The response of the sensor is affected by both the material properties of its individual components and its geometry itself. In order to set the optimal parameters for the individual components and assess the effect they have on the total response time, an automated tool based on the open source ESPRESO (Highly Parallel Solvers for Engineering Applications) library developed at IT4Innovations was created.

In order to compute the response curve required for assessing optimal functionality of the thermal sensor, it is necessary to perform tens or even hundreds of independent, computationally expensive simulations of the response. Using the ESPRESO library based on the finite element method in combination with optimal parallel algorithms, which allow the HPC infrastructure to be used to its full extent, reduces the time required for achieving optimal parameters to its minimum. Moreover, using the open source solution also minimizes the economic costs incurred when using commercial software solutions and allows the functionality to be extended to other products included in the wide portfolio of Continental Automotive Czech Republic s.r.o.



Parallel scalability of the ESPRESO library for full nonlinear time dependent problem - response time evaluation

Pavel Žáček

Mechanical Engineer Leader
BU Sensors & Actuators
Continental Automotive Czech Republic s.r.o

We highly appreciate our long-term cooperation with IT4Innovations National Supercomputing Center. Their consultations during solving complex problems are led professionally and helpfully. They are able to reflect specific impacts of the product, needs, and opportunities of our company. The achieved results presented in well-arranged reports correlate with real tested samples. The output also includes a computational model, which can be used for future optimization. We can therefore consider our cooperation with IT4Innovations to be highly productive, and we look forward to our other joint projects in the future.

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INFORMATION TECHNOLOGY CONSULTING

Partner	Bayncore
Field	information technology, consulting

At the end of 2017, our cooperation with the Bayncore company based in the UK was established, and we thus joined their partners including, for example, Intel, Microsoft, IXPUG, and Computer Laboratory – University of Cambridge (United Kingdom). Bayncore provide services in the fields of consulting and information technology. They are specialized in providing a platform for high-end technology solutions in high performance computing (HPC), technical processing of data, and big data. The Bayncore portfolio of mostly tailored services covers the following four areas: a platform for high-end IT services and consulting, research and development, training, and benchmarking. Their scope of activities covers the whole of Europe, the Middle East, and Africa (EMEA).

The very first joint project of IT4Innovations and Bayncore includes contract research and consulting services within a series of Intel AI EMEA Roadshow workshops held throughout the whole EMEA region. This partnership consists of creating machine learning related content and in co-conducting workshops in close cooperation with Bayncore and Intel. The topics covered within this cooperation include code modernization using Intel Software Development Tools, Intel optimized Deep Neural Networks and Machine Learning with Tensorflow, Caffe, and scikit-learn, and the Intel Python Distribution. From the beginning of the cooperation up to June 2018, the IT4Innovations contributions have been presented at 15 workshops.

Marc Derquennes

CEO, Bayncore

The IT4I team enriches the cooperation with Bayncore not only with expert knowledge in HPC and artificial intelligence but also with valuable hands-on experience and assistance at the meetings with experts in science. We highly appreciate IT4I's qualities, which include willingness in sharing their knowledge of designs, scientific algorithm optimization, and data analysis. IT4I participates within a project, the results of which have positive impact on the Bayncore image. The strengths of the IT4I team include precision, a professional attitude, readiness, and excellence, which are all perfect for the Bayncore company and their research and development. The cooperation with IT4I has opened the door for us to participate within a number of very interesting projects in the field of exascale/large-scale computing. IT4I also help us to fulfil our obligations, such as publishing technical papers, many-core architecture for science and research, and support of different projects in collaboration with ComputerLab of the University of Cambridge in the United Kingdom.

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