NEWSLETTER Q2/2020

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

IN BRIEF

E-INFRA CZ HAS A NEW LOGO

e-INFRA CZ is a unique e-infrastructure for research and development in the Czech Republic which we develop together with CESNETem and CERITem-SC.

TERMINATION OF ANSELM GUARANTEE SUPPORT

The guarantee support for Anselm from its supplier was terminated on 18th May 2020. Since then Anselm has been operated in maintenance mode, and will be until the end of the year 2020. During this period we are no longer able to fully guarantee the security and consistency of the data stored. We strongly recommend that you store confidential data somewhere else.

For more information, do not hesitate to contact our support via support@it4i.cz

A PAPER ABOUT THE READEX PROJECT HAS ACHIEVED SUCCESS

The paper titled Domain Knowledge Specification for Energy Tuning, which was co-authored by our colleagues Lubomír Říha, Ondřej Vysocký, Martin Beseda, and Jan Zapletal, ranks among the 10 % most frequently downloaded contributions in Concurrency and Computation: Practice and Experience.

Read the article

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content

IN BRIEF

SUMMER OF HPC IS KICKING OFF

Another round of Summer of HPC hosting three students is kicking off at IT4Innovations. Marco Mattia and Denizhan Tutar will work on the project titled Development of a visualization tool for data from molecular simulations, under the supervision of Martin Beseda and Rajko Cosic. Andres Vicente Arevalo, on the other hand, will work on the project titled Object Detection Using Deep Neural Networks – AI from HPC to the Edge, under the supervision of Georg Zitzlsbergr and Martin Golasowski. As any other events, this year's Summer of HPC could not be saved from the coronavirus mitigation measures, and therefore it is taking place virtually.

EOSC LANDSCAPING WEBINAR

On June 23, e-INFRA CZ organized a webinar dedicated to the European Open Science Cloud (EOSC) as well as to EOSC Landscaping and its results in the Czech Republic. At the webinar, information about the current situation and direction of the EOSC were provided. The main topics introduced were the results of the EOSC survey among Czech research infrastructures, e-infrastructures, and science donors.

See the presentation HERE

LUMI HAS A NEW WEBSITE

A brand new website of the LUMI consortium, in which IT4Innovations plays a part, has been launched.

https://www.lumi-supercomputer.eu/
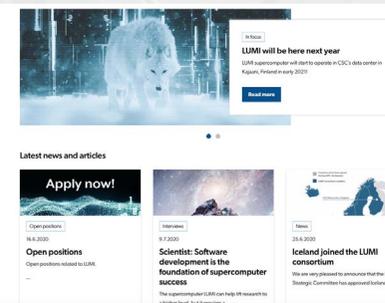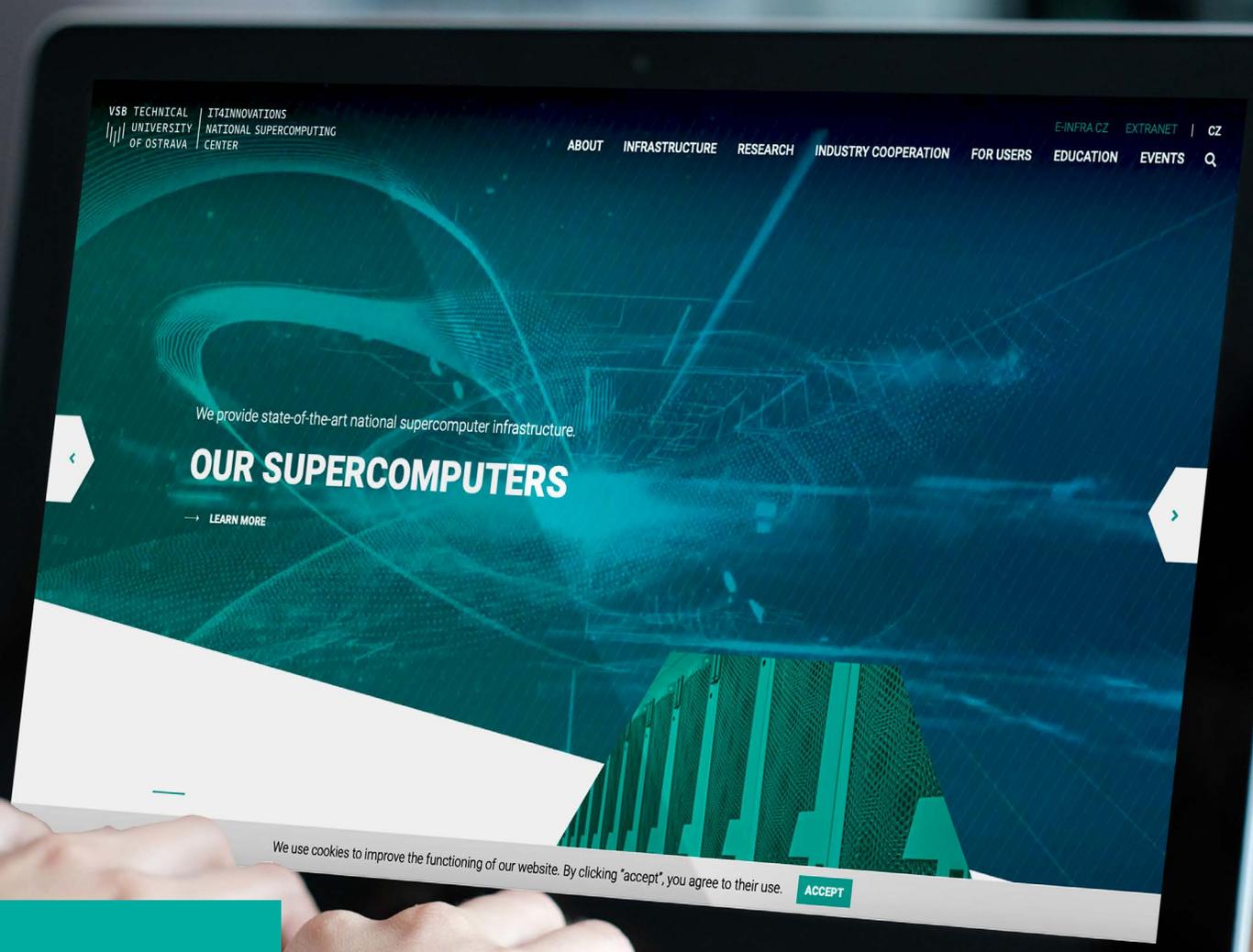
A BRAND NEW IT4INNOVATIONS
WEBSITE HAS BEEN LAUNCHED

A brand new IT4Innovations website has been launched

In June, our new web presentation in both Czech and English was launched. You can visit our website using the link **www.it4i.cz**. Not only the website design but also its content has gone through a significant evolution. The new website is fully responsive and available on mobile devices.

Extranet and **Docs** addresses as well as access to our **HelpDesk** are still valid.

We believe that the simplified finding of needed information on our new website will make your work easier.

In the main sections, you can find this information, among others:

• **ABOUT IT4I** – publications, press releases, organizational structure, memberships, etc.,

• **INFRASTRUCTURE** – detailed information about our existing and planned clusters as well as operating technology,

• **RESEARCH** – information about currently implemented projects of IT4I and our users,

• **INDUSTRY COOPERATION** – a portfolio of our services provided to our industrial partners and examples of cooperation with them,

• **FOR USERS** – how to obtain computational resources; open access calls including all necessary documents and forms,

• **EDUCATION** – educational activities, our doctoral study programme, and the Doctoral School,

• **EVENTS** – for the scientific community, our users, and the general public.
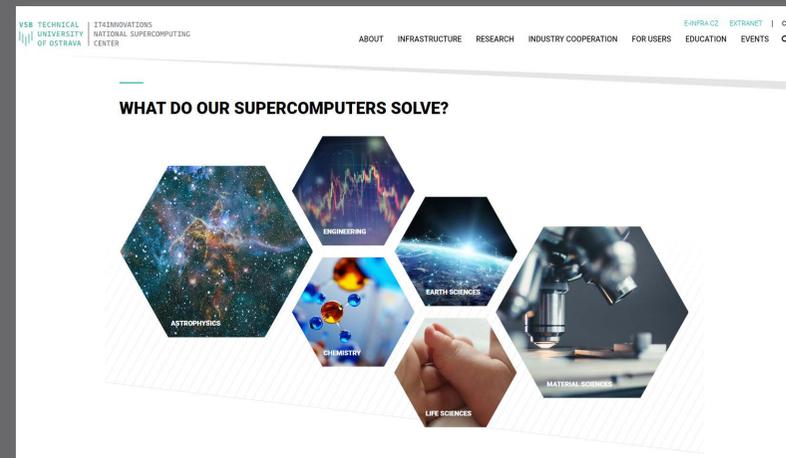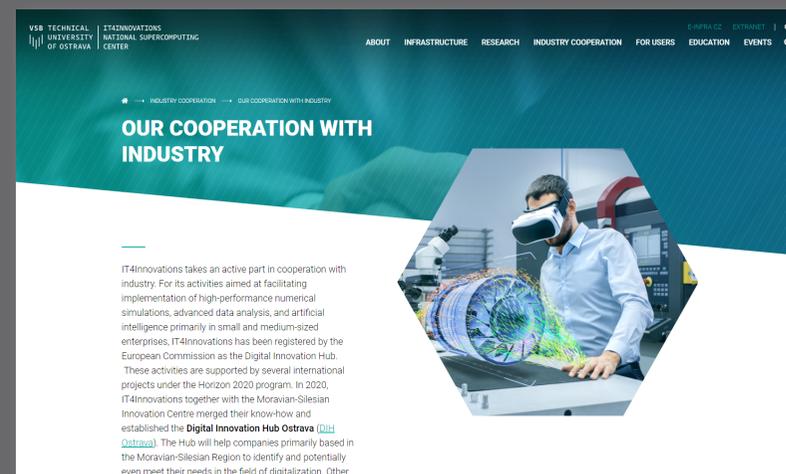
www.it4i.cz

Rethinking the stellar explosions that mark cosmic distances p. 1046

Mangrove survival in rising seas pp. 1050 & 1118

Next-generation fluorocarbons in the environment pp. 1066 & 1103

Science

$15
5 JUNE 2020
sciencemag.org

AAAS

METALLIC
SOLUTION

Electrolyte-to-metal
transition of electrons dissolved
in ammonia pp. 1056 & 1086

WE HAVE CONTRIBUTED TO
A RESEARCH PROJECT WHICH IS
ON THE COVER OF THE MAGAZINE SCIENCE

We have contributed to a research project which is on the cover of the magazine Science

The research team led by Pavel Jungwirth from the Institute of Organic Chemistry and Biochemistry (IOCB) of the CAS and their project has made it onto the cover of one of the most prestigious and cited scientific magazines worldwide: Science. It is an honour for us that IT4Innovations also took the opportunity to contribute to this invention by granting 650,000 core hours of its computational resources to Pavel Jungwirth for his research.

The article published in Science magazine is titled Photoelectron spectra of alkali metal-ammonia microjets: From blue electrolyte to bronze metal, and answers the question of what metal is and how it is actually formed. In cooperation with his colleagues from the IOCB and scientists from the Czech Republic, Germany, and the USA, Pavel Jungwirth made use of advanced electron structure calculations and photoelectron spectroscopy (PES), described, and at the molecular level mapped electrolyte-to-metal transition in alkali metal–liquid ammonia solutions.

Alkali metals dissolved in liquid ammonia represent archetypal systems to explore the transition from blue electrolytes at low concentrations to bronze or gold colored metallic solutions (with conductivity comparable to a copper wire) with higher concentrations of excess electrons. At the same time, PES represents an ideal tool for establishing the electronic structure pertinent to this transition.

As an ultra-high vacuum technique, PES was long thought to be incompatible with volatile liquids until the technique of liquid microjets was developed for water and aqueous solutions. However, it was only in 2019 that the group of Pavel Jungwirth, in collaboration with colleagues at the University of Southern California and at the BESSY II synchrotron in Berlin, performed the first successful PES measurements on pure liquid ammonia.

"This achievement has opened the door to further studies of alkali metal – liquid ammonia systems using photoelectron spectroscopy and led to the latest Science publication, which maps the electrolyte-to-metal transition for lithium, sodium, and potassium dissolved in liquid ammonia by means of photoelectron spectroscopy. Hopefully the present work on metallic ammonia will open the path to realizing our most 'explosive' idea: The preparation of metallic water by very carefully mixing it with alkali metals," concludes Pavel Jungwirth.

By employing photoelectron spectroscopy using soft x-ray synchotron radiation, the researchers captured for the first time a photoelectron signal around 2 eV binding energy corresponding to electrons dissolved in liquid ammonia. With increasing alkali metal concentration the transition to metallic behaviour appears in the photoelectron spectrum by creating a conduction band with a sharp Fermi edge accompanied by plasmon peaks.

Together with state-of-the-art electronic structure calculations co-performed by experts from the Faculty of Mathematics and Physics of Charles University in Prague, these measurements provide a detailed molecular picture of the transition from a non-metal to a metal, allowing us to better understand the onset of metallic behavior characterized by properties such as very high electric conductivity.

Read the article HERE
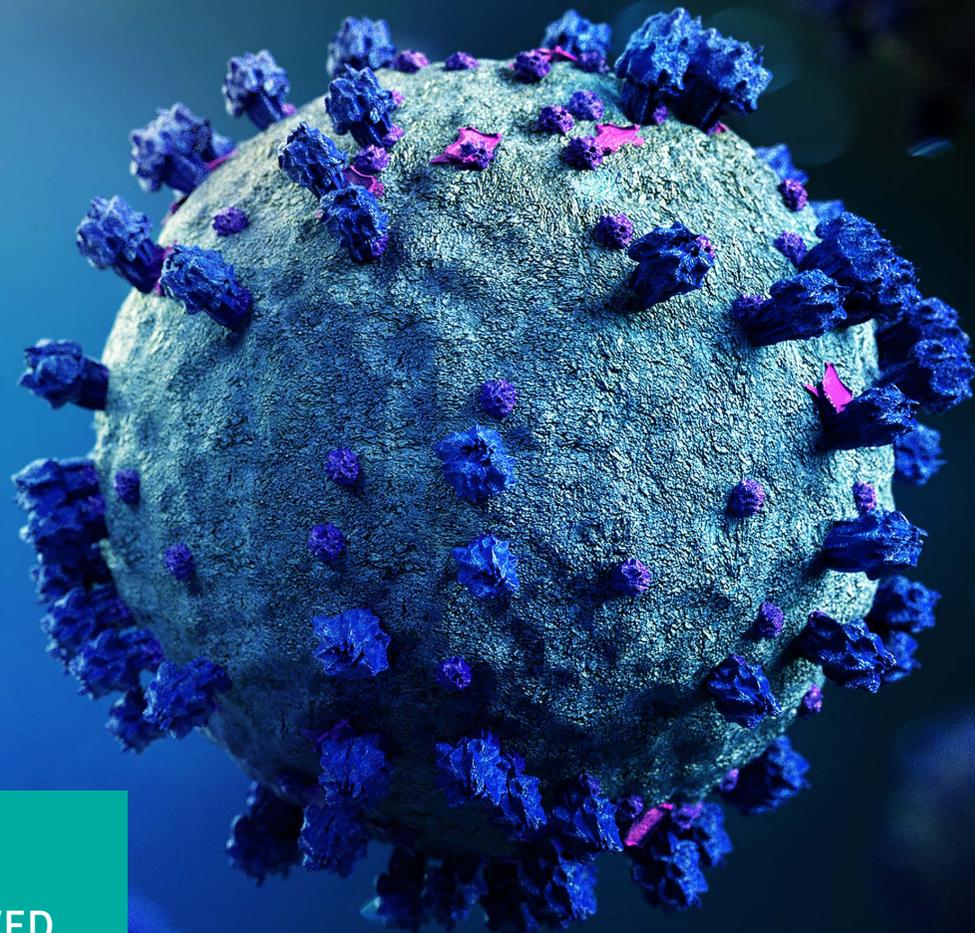
WE HAVE BECOME ACTIVELY INVOLVED
IN COMBATTING COVID-19

We have become actively involved in combatting COVID-19

In recent months, coronavirus has paralyzed the economy of many countries, has caused the collapse of many health institutions and left hundreds of thousands of deaths behind. A number of scientists are now focused on searching for medication that would cure people infected with the disease COVID-19. However, the process of discovering new medication is very expensive and the medication reaches the market after many years of testing. This problem can be helped by supercomputers which manage to boost the testing significantly and thus reduce the investment. IT4Innovations is also involved in activities to help fight the coronavirus.

Priority access to IT4Innovations computational resources

Immediately after the outburst of the pandemic in the Czech Republic, IT4Innovations responded to the actual situation and offered its users priority access to its computational resources to solve problems regarding the COVID-19 disease research. *"We have called on our users to apply for our computational resources provided that they are currently involved in research addressing the COVID-19 disease. They can do so by submitting the application, which will be immediately approved and given priority access to our computational resources. Projects to be supported do not necessarily need to be focused only on drug design but could include development of nanomaterials or pandemic spread mo-*

delling among others," says Vit Vondrak, IT4Innovations Managing Director. IT4Innovations computational resources were also offered to be used for the initiative of the European Commission **EUvsVIRUS Hackathon**, which took place from 24th April to 26th April. The aim of the cross-European hackathon was to develop an innovative solution to overcome the social challenges connected with the coronavirus.
More information at https://euvsvirus.org

Mobility atlas

Another significant project, carried out by the Advanced Data Analysis and Simulation Lab led by Miroslav Vozňák, is the Mobility Atlas. It is a primary data passing interface to monitor population mobility in the territory of the Czech Republic during the state of emergency processed from anonymous operating data collected by T-Mobile CZ using the services of IT4Innovations. Our supercomputers are currently processing aggregated anonymized records from the mobile network and provide population mobility data at the most granular territorial level. *"Under the instructions of T-Mobile Czech Republic, we are creating access to the mobility portal where various sets can be generated based on the roles assigned. All has been running autonomously and smoothly so far despite our constant intervention and customized adjustment of data views,"* explains Miroslav Vozňák.
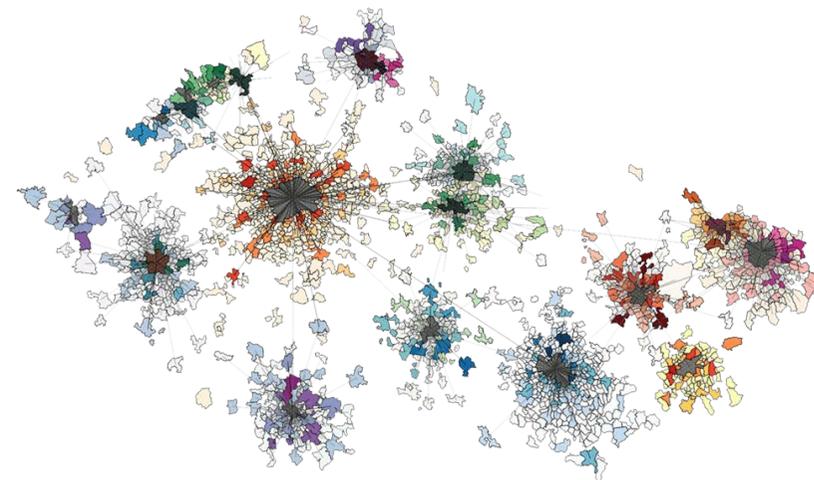
Mobility atlas

Cooperation with Politecnico di Milano in the search for medication against coronavirus

IT4Innovations has again started cooperation with Politecnico di Milano, Italy and offered a hand in research regarding the most discussed disease of this time – COVID-19. *"Within this cooperation, novel algorithms and methods for the discovery of a therapeutic solution against coronavirus will also be tested on our supercomputers. The main aim of this research is to prepare the ground for a quick response in case of a pandemic, while for the future the utilization of the LEXIS platform is accounted for, which combines the advantages of high-performance computing, cloud and operating large data files. LEXIS will enable the testing of algorithms across various supercomputing centers, which will lead to experiments on a large scale,"* stated Jan Martinovič, the Head of Advanced Data Analysis and Simulations Lab at IT4Innovations and the Coordinator of the LEXIS project.

IT4Innovations is the only Czech representative in the prestigious Exscalate-4COV League

The members of Exscalate4COV League, which also involve IT4Innovations, are actively working on searching for medication against the coronavirus. Industrial and scientific entities, which are not a formal part of the consortium, are also involved, contributing with material, knowledge and other resources in this project.
 "Within the project Exscalate4COV, an initial investigation on the reduced database of 10, 000 available drugs has been already done, and currently the challenging part is to extend it to more than 500 billion molecules. Here is where supercomputers make the difference by supporting a fast selection of only the most promising molecules to be sent to the subsequent phases of the drug discovery pipeline. The experience we had in the ANTAREX project with IT4Innovations was successful and the current collaboration can help us in further accelerating the computational process for facing a future pandemic," said Gianluca Palermo, Politecnico di Milano principal scientist in the Exscalate4COV project.

EXSCALATE 4COV

More information HERE

WE INTRODUCE THE NEW
VIARODOS APPLICATION

We introduce the new viaRODOS application

IT4Innovations National Supercomputing Center presents an updated viaRODOS application, which was developed within the RODOS project, and cooperates with the Floreon+ system. The application uses data sources provided by the National Traffic Information Center (NDIC), which falls under the Directorate of Roads and Motorways of the Czech Republic. Users thus receive the most up-to-date data on traffic on roads and in selected cities in the Czech Republic.

Fourteen years ago, research teams at VSB – Technical University of Ostrava developed the Floreon+ application to evaluate information for decision making in crisis management processes, especially floods. This year, researchers at IT4Innovations National Supercomputing Center have upgraded the viaRODOS application, developed within the RODOS Transport Systems Development Center, and connected it to the Floreon+ system. An impor-

tant part of the modernization is the connection to new data sources from the area monitoring telematics system (FCD) acquired by the Directorate of Roads and Motorways of the Czech Republic.

Users, especially drivers, are brought a new upgraded viaRODOS application, which is accessible via the web interface at www.viarodos.cz, and current data on traffic not only on highways and roads in the Czech Republic but also closures and traffic restraints in selected cities, all in real time.

IT4Innovations is now becoming the new viaRODOS operator.

"I am very pleased that the projects that were created at VSB – Technical University of Ostrava many years ago find use even after such a long time. The modernized viaRODOS application will find wide application not only among Czech citizens but also among experts in the field of crisis management," says Ivo Vondrák, the Governor

of the Moravian-Silesian Region, who was also the Rector of VSB – Technical University of Ostrava at the birth of the Floreon+ application.viaRODOS shows the current traffic situation on selected roads in the Czech Republic, with the help of simple line graphics as well as a map visualization with data update at one-minute intervals. It is interesting to note that data from the viaRODOS application is also actively used by Czech Television in its news coverage.

"I believe that the cooperation between VSB and ŘSD in the field of telematics and the processing of traffic big data will continue to develop. The FCD project is proof that the results of science and research can be successfully translated into practice. We are all the more pleased with the fact that the information from the area monitoring telematics system has returned to academia and will certainly find other uses than just the basic display on the map. For the sake of completeness,

let us add that information from an area telematics source, similar to traffic information, is available free of charge from NDIC to all customers in the form of open data," says Filip Týc, Head of the Road Databank and NDIC Department, who participated in the presented project.

"We took over the viaRODOS application at IT4Innovations under our administration this January and connected it with the new data sources of the National Traffic Information System. As part of the application update, there was also a connection with the Floreon+ system, which allows us to improve the capabilities of the viaRODOS application in the area of telematics data visualization within the map base. The user can also look at the development of the traffic situation over time," adds Jan Martinovič from IT4Innovations, whose team from the Advanced Data Analysis and Simulation Lab administers the application.

A BRIEF NOTE ABOUT
THE VIARODOS APPLICATION

The main page shows an overview of the main roads in the Czech Republic, for which more detailed visualizations are created on separate pages. The application menu allows the user to move between other menus showing the current traffic situation in selected cities in the Czech Republic. At the top of the screen is a black bar with the name of the current page and the time remaining until the next automatic update.

The application provides two types of traffic information:

· Line graphics – the option by clicking on the menu "Main road routes" allows a preview of the overall traffic situation on selected routes and displays the current situation in the form of a general overview. The route captures either one specific road or a traffic lane between the start and the end point, which consists of several road sections. The details of the route then display more detailed information such as the speed of the traffic flow, delays on individual sections, traffic restrictions, etc.

· Map information – after selecting the Czech Republic or clicking on the city name, the map using the Floreon+ application will be displayed. The main roads in the Czech Republic embedded in the map provide a quick overview of the overall traffic situation with the possibility of displaying the history of the situation by means of the timeline in the Floreon+ application. The application also allows the user to set the display of different layers with traffic information.

GIVE OUR NEW SERVICE TO SUPPORT
RESEARCH AND DEVELOPMENT A TRY

Give our new service to support research and development a try

The POP2 project, which is an acronym for Perfor¬mance Optimisation and Productivity 2, follows the successfully implemented POP project, which started in 2015. By means of the POP2 project, IT4Innovations offers a service to support research and development within the international Centre of Excellence project. It is free of charge assistance in the field of parallel applications optimization. The service is designed not only for all scientists and researchers but also for employees of companies who develop and use parallel codes and tools, and would welcome expert assistance with their optimization for efficient running on powerful supercomputers.

"The main activity within the POP2 project is to assist in analysing parallel applications, identifying bugs in codes, and proposing optimization methods leading to higher performance and enhanced scalability of a given application," specifies Lubomír Říha, the Head of the Infra-

structure Research Lab and the Principal Investigator of the POP2 project.
The Centre of Excellence for Performance Optimisation and Productivity in computational applications has received funding from the European Commission to detect inefficiencies and their causes in parallel codes. The first phase of the project was successfully completed in March, with a total of 158 resolved cases when a large number of parallel applications was verified. The second phase of the project commenced in December 2018 and will take three years to complete.

For more information about the project and particular examples of successful implementations, see the following website: https://pop-coe.eu/. These services are free of charge for all organizations residing in the European Union so do not hesitate and in case of interest contact us using the following e-mail: info@it4i.cz.

POP2 (PERFORMANCE OPTIMISATION AND PRODUCTIVITY 2) PROJECT

- **2018 to 2021**

- **Funded by the European Union Horizon 2020 programme**

- **8 partners: BSC (Spain), Universitaet Stttutgart (Germany), Forschungszentrum Jülich (Germany), RWTH Aachen (Germany), Numerical Algorithms Group (UK), Teratec (France), University Versailles Saint Quentin en Yvelines (France), and VSB-TUO / IT4Innovations National Supercomputing Center (Czech Republic)**

More information about the POP2 project HERE
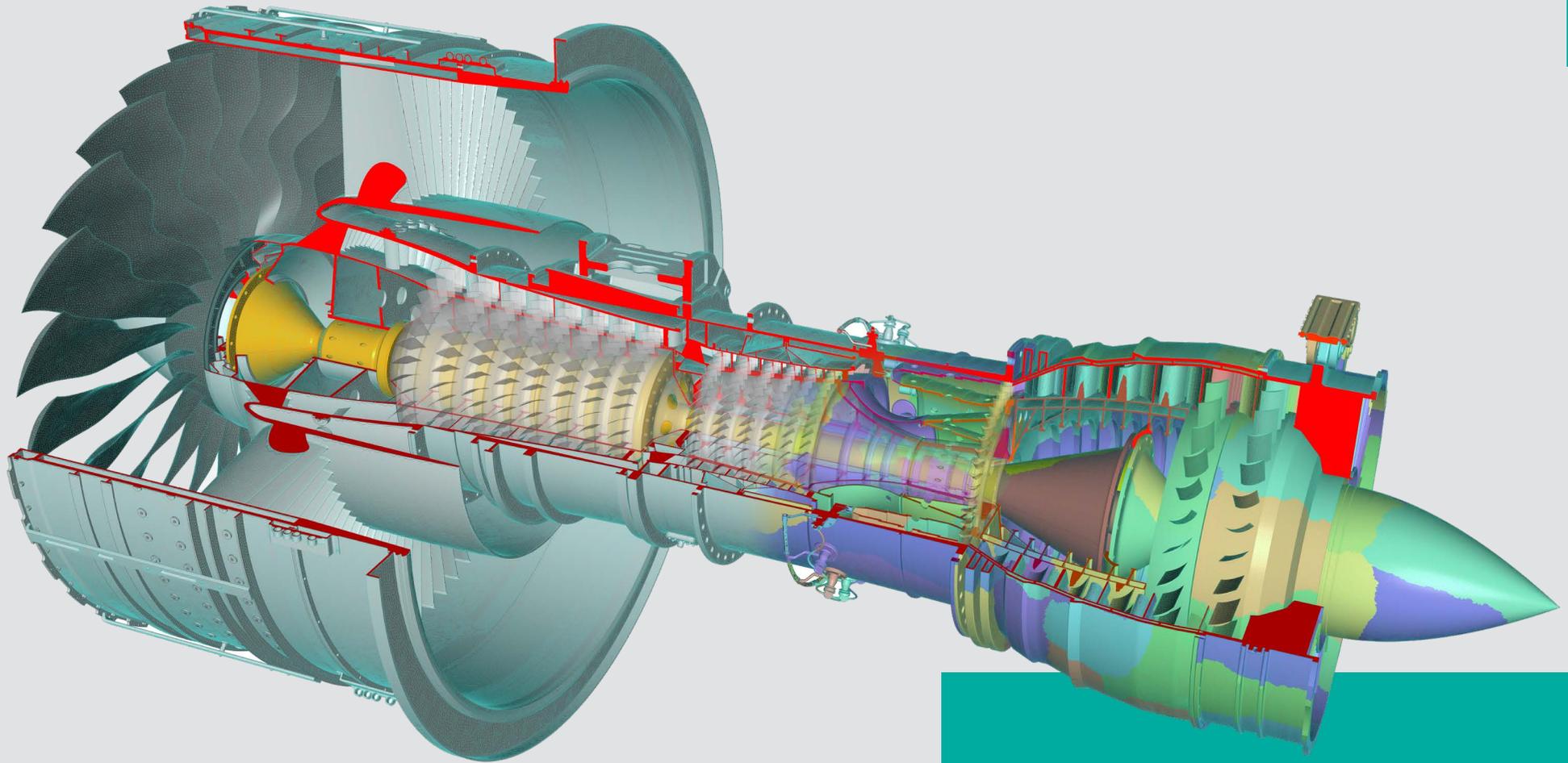
ESPRESO – MASSIVELY PARALLEL LIBRARY
FOR ENGINEERING APPLICATIONS

The latest advances in IT technology have brought about a significant change in the concept of new product design, production management, and autonomous systems. In the last few years, we have witnessed a significant transition to virtual prototyping, and gradually increasing pressure for the integration of a large part of the industrial sector towards the new industrial revolution, otherwise known as Industry 4.0. Therefore, the IT4Innovations (IT4I) research labs offer their expertise and experience with development and implementation of new parallel methods and algorithms for computationally intensive numerical simulations in mechanical engineering, civil engineering, biomechanics, and the energy industry.

Let supercomputers save you time and discover deeper possibilities for your product design

Within its research activities, IT4I develops the open--source ESPRESO simulation package. It is designed to solve complex engineering problems, and during its development, emphasis is placed on optimal use of high-performance computing infrastructure (HPC). The package is distributed based on a free of charge open-source licence, which makes the application of automated simulation chains, such as computing templates customized to suit the specific product portfolio, significantly easier, and is useful for easy performance of multiple calculations without any licence fees or liabilities. Since the very beginning, each module within

the software package is developed as a parallel code based on massively scalable numerical methods and algorithms. Thereby we are able to ensure optimal utilization of state-of-the-art supercomputers. The added value of the package is our implementation of a FETI domain decomposition-based massively parallel linear solver, which is able to solve problems of hundreds of billions of unknowns.

The package contains several logical units, which can be combined to reflect particular requirements for a given problem solution. These units include entry data preprocessing, computational mesh processing, numerical model construction, specific physical problem solution using a massively parallel sparse linear solver in combination with available nonlinear solvers, and final preparation of output data for visualization and online monitoring of achieved results. Another key property of the package is its simple and flexible configuration interface, by means of which all modules can be controlled using single configuration. This interface can be extended easily, and its simple form allows it to be interconnected via a web portal with the HPC-as-a-Service system, which is being developed by the IT4I Advanced Data Analysis and Simulation Lab. HPC-as-a-Service is a well-known term in the field of High-Performance Computing systems, meaning users can access an HPC infrastructure with no need to buy and administer their own physical servers or

data centre infrastructure. Via this service, users have an opportunity to use HPC technologies without any prior investment into hardware. Moreover, this access further reduces the entry barrier for users and small and medium-sized enterprises who are interested in utilization of massively parallel computers, but often lack the necessary knowledge level. You can learn more about this service in the next issue of our Newsletter or on our website, where our HPC platform for scientific workflow flagship is to be presented.

ESPRESO – KEY PROPERTIES

- a complex open-source finite element solver for HPC infrastructure,
- interconnection with popular commercial as well as open-source tools,
- scalable solvers for the most powerful supercomputers,
- a simple interface for automated solutions.

More information about the ESPRESO library HERE

ESPRESO – FAST AND SCALABLE INPUT

The I/O module of the ESPRESO package is designed so as to efficiently load database files containing unstructured computational meshes and perform high-quality domain decomposition. It is conceptualy developed as a massively parallel tool designated for the HPC environment, including high-performance storage systems.
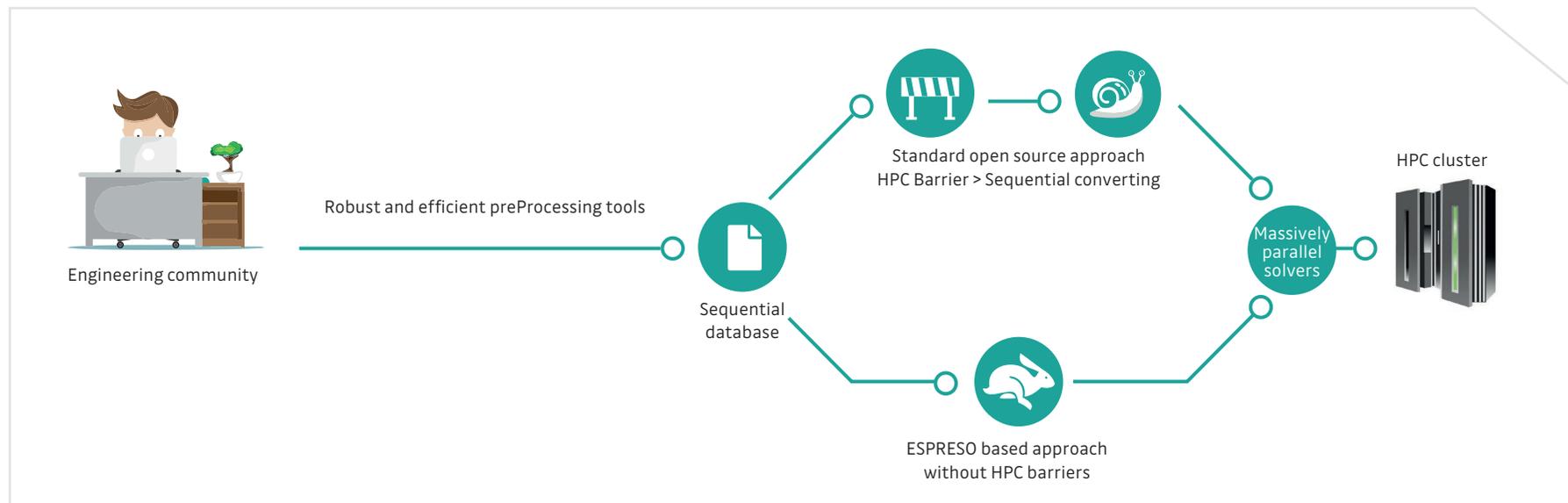
In developing the I/O module, our motivation was to interconnect tools for creating complex engineering models such as ANSYS, HyperMesh, ANSA, ABAQUS, and open-source parallel solvers. This direct interconnection allows not only wider use of HPC technologies without any additional costs of commercial licences in the case of repetitive calculations or solving non-standard problems, but also use of robust commercial pre-processing tools for preparation of complex

sets in cases where excessive demands on computational mesh quality are required.

The module can be used in two ways, either as a parallel convertor for various formats, or as a direct loader and pre-processor of massively parallel solvers of the ESPRESO package. In the latter case, the user can use a database file saved in his/her favourite format and use it for multiple calculations. Every calculation can be performed using a different number of compute nodes without further restrictions as our approach does not require running on a fixed number of MPI processors and domains as in the case of a parallel binary file. This solution allows a different amount of computational resources to be used based on the needs or availability of computational resources.

Supported input formats:

- ANSYS CDB
- EnSight
- VTK
- XDMF
- OpenFOAM
- Abaqus

Robust and efficient preProcessing tools

Engineering community

Sequential database

Standard open source approach
HPC Barrier > Sequential converting

ESPRESO based approach
without HPC barriers

Massively parallel solvers

HPC cluster

Parallel loading of unstructured meshes

- direct input into the parallel solver without the need for conversion of a database file,
- support for various formats containing unstructured meshes (support for a new format easily implementable based on user demands),
- restart of a calculation using a different amount of allocated resources.

Domain decomposition

- geometric decomposition based on the Hilbert space-filling curve,
- connection to state-of-the-art graph decomposition libraries with significant improvement of its parallel scalability.
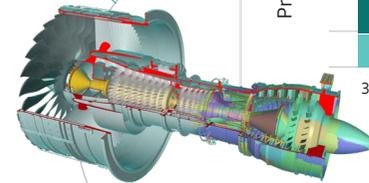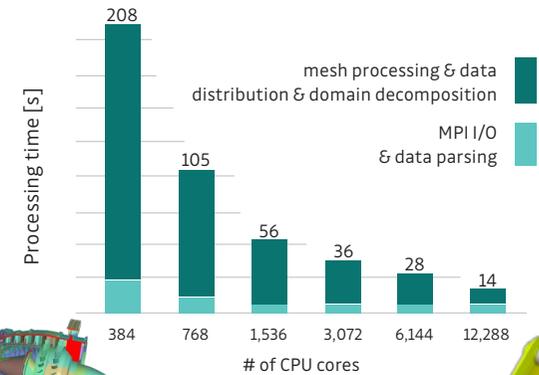
Asynchronnous output

- overlapping of running calculations by storing solution results,
- output to commonly used postprocessing formats such as EnSight and VTK,
- monitoring of results on selected regions for statistic and optimization toolchain,
- restart of solutions without any connection to a previous amount of computational resources.
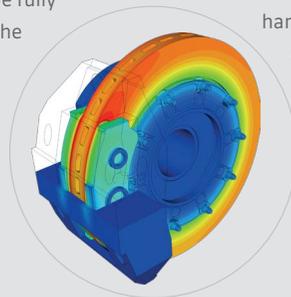
Jet engine

- Sequence database file – size of 150 GB
- Mesh downloaded and decomposed in 14 seconds
- 822 million computing points
- 12 288 CPU cores

## WHOLE WORKFLOW STRONG SCALABILITY TEST JEN ENGINE

Legend:
- mesh processing & data distribution & domain decomposition
- MPI I/O & data parsing

Processing time [s]

Values: 208, 105, 56, 36, 28, 14

# of CPU cores: 384, 768, 1,536, 3,072, 6,144, 12,288

ESPRESO – FEM LIBRARY

One of the main parts of our product is a complete FEM module for description of physical processes. Development of this module follows from IT4I collaboration with industrial partners as well as implemented national and international projects. All parts of the FEM module contain massively scalable methods, which allow the computational capacity of the state-of-the-art supercomputers to be fully utilized. One of the complete modules of the FEM library is, for example, a module for heat transfer problems. This module is designed to solve complex engineering problems while covering all physical aspects such as convection, conduction, radiation, and advection, which are related to nonlinear and time-dependent problems. A simple configuration interface allows combining both steady state and time-dependent analyses.

The module for solving problems of structural mechanics includes nonlinear material models, contact problems, harmonic response analysis, implicit time schemes, and others. By combining mesh morphing using RBF (Radial Basis Function), internal scalable solvers, and modular configuration, an optimal design can be created in a short time.
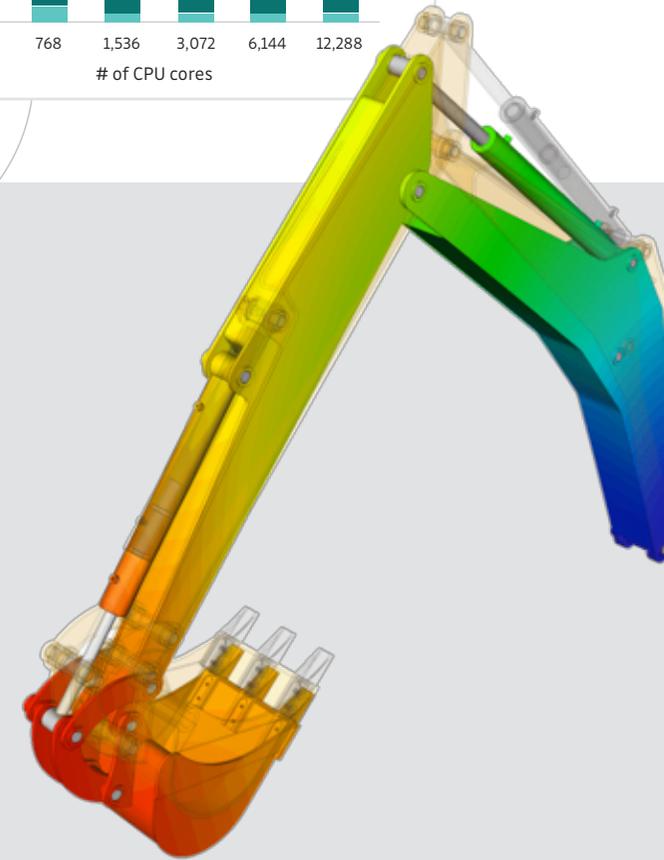
ESPRESO – MASSIVELY PARALLEL SOLVER

The ESPRESO library contains several massively scalable solvers, which are based on domain decomposition methods developed by an in-house research group, allowing the computational capacity of the state-of-the-art supercomputers to be fully utilized thus being able to solve problems with hundreds of billions of unknows.

- The in-house massively parallel solver based on multilevel FETI domain decomposition methods allows solving problems with billions of unknowns,
- CPU version for massively parallel systems,
- a version offering utilization of NVIDIA GPU accelerators,
- quadratic programming methods to solve contact problems,
- automated tuning of the solver setting using evolutionary algorithms.

Successfully tested on large petascale systems:
- Titan – Oak Ridge National Laboratory, USA
- Piz Daint – CSCS, Switzerland
- Salomon – IT4Innovations, Czech Republic

Available third-party solvers
In the case of highly heterogenous systems, parallel direct solvers or algebraic multigrid can be used to solve defined problems.

Principal authors of the ESPRESO library:
Lubomír Říha, Ondřej Meca, Tomáš Brzobohatý, Oldřich Vlach, and Alexandros Markopoulos.

STRONG SCALABILITY - STRUCTURAL MECHANICS BENCHMARK

FETI/HFETI
300 Million unknowns

Solver runtime [s]

683, 369, 195, 87, 34

552, 1,128, 2,232, 4,464, 8,928
# of CPU cores of Salomon Supercomputer
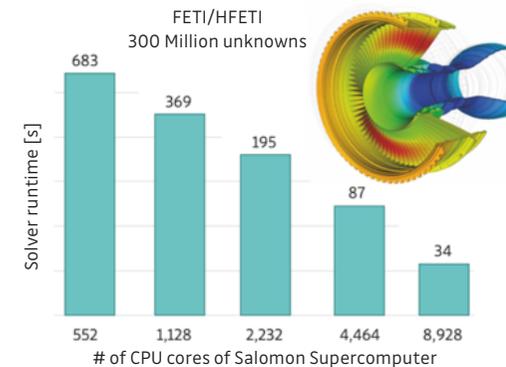
STRONG SCLABILITY – UNIFORM BENCHMARK

Solver runtime [s]

11 billion unknowns
Linear elasticity problem

20 billion unknowns
Heat transfer problem

139, 221, 82, 135, 52, 83, 40, 59, 30, 40, 18, 22

43,904, 65,536, 93,312, 128,000, 170,368, 281,216
# of CPU cores of Titan Supercomputer

Input from external
pre-processing tools

ESPRESO

Output to external
post-processing tools

Fast and Scalable
Input/Output

Mesh Morphing

Finite
element library

Σ

Massively
Parallel Solvers

Automatized
simulation chains
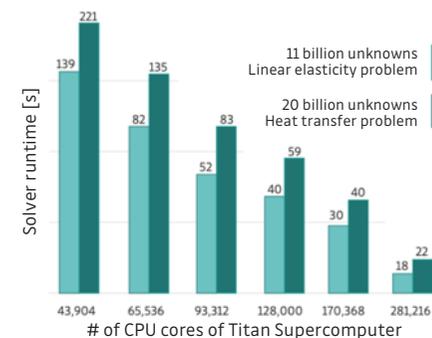
NEWLY PROCURED SOFTWARE TO FACILITATE THE WORK OF OUR USERS

Since 2017, the IT4Innovations national supercomputing center – path to exascale project has been running. The main objective of the project is to extend and modernize the IT4Innovations research infrastructures so as to at least maintain the existing technology level of HPC in the Czech Republic in comparison with developed, primarily European, countries. In 2019, this project led to extending the computational capacity of our centre with the Barbora supercomputer, which will gradually replace Anselm, the very first IT4Innovations supercomputer. In 2020, a new supercomputer with multiple times the performance of Salomon, the current most powerful IT4Innovations system, will be procured.

Within the project, high-quality research of the wider scientific community in the Czech Republic as well as broadening of the existing research activities at IT4Innovations are also supported. For the IT4Innovations infrastructure, in-house research is an important source of HPC expertise, which is reflected in the services provided by the infrastructure to its users. Therefore, new software packages have been procured within the project to help not only the IT4Innovations researchers and IT specialists but also the research infrastructure users. We bring you a list of the procured software packages and their main advantages.

ALLINEA FORGE

Allinea Forge consists of two tools: **Allinea DDT** is a commercial debugger primarily for debugging parallel MPI or OpenMP programs. It also supports GPU (CUDA) and Intel Xeon Phi accelerators. DDT provides all the standard debugging features for every thread running as a part of your program, or for every process - even if these processes are distributed across a cluster using an MPI implementation. **Allinea MAP** is a profiler for C/C++/Fortran HPC codes. It is designed for profiling parallel code which uses pthreads, OpenMP, or MPI.

TOTALVIEW

The Top HPC Debugger for Research Computing. The TotalView debugging software provides specialized tools necessary for quick debugging, analysis, and scaling high--performance computing (HPC) applications. This includes highly dynamic, parallel, and multicore applications that run on diverse hardware, from desktops to supercomputers.

CST STUDIO SUITE

This is a high-performance 3D EM analysis software package for designing, analysing, and optimizing electromagnetic (EM) components and systems. CST Studio Suite is used in leading technology and engineering companies around the world. It offers considerable product to market advantages, facilitating shorter development cycles and reduced costs. Simulation enables the use of virtual prototyping. Device performance can be optimized, potential compliance issues identified and mitigated early in the design process, the number of physical prototypes required can be reduced, and the risk of test failures and recalls minimized.

MOLPRO

MOLPRO is a complete software package used for accurate ab-initio quantum chemistry calculations. The emphasis is on highly accurate computations, with extensive treatment of the electron correlation problem through the multiconfiguration-reference CI, coupled cluster, and associated methods. Using the recently developed integral-direct local electron correlation methods, which significantly reduce the increase of the computational costs with moelcular size, accurate ab initio calculations can be perfomed for much larger molecules than has previously been possible.

Detailed information about the installed software package HERE

MEDEA

The MedeA software package is the leading environment for atomistic simulation of materials. MedeA enables professional, day-to-day deployment of atomic-scale and nano-scale computations for materials engineering, materials optimization, and materials discovery. In MedeA, world-class simulation engines are integrated with elaborate property prediction modules, experimental databases, structure builders, and analysis tools, all in one user-friendly environment.

GAUSSIAN

Gaussian is the latest version of the Gaussian series of electronic structure programs, used by chemists, chemical engineers, biochemists, physicists, and other scientists worldwide. Gaussian provides a wide-ranging suite of the most advanced modeling capabilities available. TCP Linda is a parallel execution environment, which has been used to create a parallel version of Gaussian for local area network and some distributed memory multiprocessor environments.

PGI PROFESSIONAL EDITION

This enables the development of performance-portable HPC applications with a uniform source code across the most widely used parallel processors and systems. PGI Professional Edition is a perpetual license to current and all previous releases of the PGI Fortran, C and C++ compilers and tools for multicore CPUs and NVIDIA Tesla GPUs, including all OpenACC, OpenMP and CUDA Fortran features.

SCHRÖDINGER MS SUITE

A platform that powers the design of novel materials in a wide array of industries, including aerospace, energy, semiconductors, and electronic displays. Molecular simulation can accelerate the development of new materials by helping you identify the most promising structures and compositions before you begin synthesis and testing.

INTEL PARALLEL STUDIO XE CLUSTER EDITION

This enables development of high-performance parallel codes and can accelerate workloads across company, cloud, high-performance computing (HPC) and Artificial Intelligence applications. This comprehensive suite of development tools makes it simpler to build and modernize codes with the latest techniques in vectorization, multithreading, multinode parallelization, and memory optimization. It enables C, C++, Fortran, and Python software developers to create faster codes, build codes faster, and obtain Priority Support.

TURBOMOLE

A collaborative, multi-national software development project aiming to provide highly efficient and stable computational tools for quantum chemical simulations of molecules, clusters, periodic systems, and solutions.

NEW INFRASTRUCTURE TO
SIGNIFICANTLY FACILITATE IMPLEMENTATION
OF THE LEXIS PROJECT

New infrastructure to significantly facilitate implementation of the LEXIS project

The LEXIS project, coordinated by IT4Innovations, creates an advanced technology platform which uses the geographically distributed computational resources of the existing European supercomputing infrastructure for big data analytical solutions and extends it with cloud services. The main objective of the mentioned H2020 project, funded by the European Union, is to use state-of--the-art resources for ensuring successful convergence of supercomputing and cloud technologies.

The LEXIS project consortium, comprising important European supercomputing centres, industrial enterprise representatives, and technology providers, is successfully advancing in solving the research objectives defined within the project, primarily thanks to smooth cooperation among the partners, and new infrastructures installed at IT4Innovations National Supercomputing Center in the Czech Republic and Leibniz Rechenzentrum (LRZ) in Germany.

"The most important part of the infrastructure includes Burst Buffer servers, which provide 24 TB of very fast NVMe storage. The new servers are also equipped with Intel Cascade Lake processors and 1 TB of experimental NVDIMM memory. The mentioned device provides very fast storage for big data processing using cloud as well as supercomputing infrastructure technologies," says Jan Martinovič, the

LEXIS project coordinator and Head of the Advanced Data Analysis and Simulation Lab at IT4Innovations.

Burst Buffer servers are part of the solution implemented by the ATOS company, which is the technology provider as well as a LEXIS project partner. Both supercomputing centres, IT4Innovations and LRZ, installed two Burst Buffer servers. Moreover, one of the servers located at IT4Innovations is also equipped with the Bittware 520N acceleration card containing FPGA Intel Stratix 10. The card will be used, for example, for on-line compression, acceleration of computationally intensive tasks, and big data processing.

In addition, IT4Innovations also obtained and launched a cloud infrastructure comprising the 120 TB CEPH storage, and 6 virtualization nodes providing a total of 240 processor cores and 1.2 TB RAM. The infrastructure is interconnected with a 100 Gbit/s Ethernet network built on the technology provided by the Mellanox company. The virtualization infrastructure will be used to operate the OpenStack cloud software. The new infrastructure will be used to operate an experimental orchestration platform, which is being developed within the LEXIS project. The platform will make use of the Ystia Orchestrator software provided by ATOS, which makes processing of complex scientific workflows within the LEXIS platform easier and more efficient.

More about the LEXIS project HERE

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