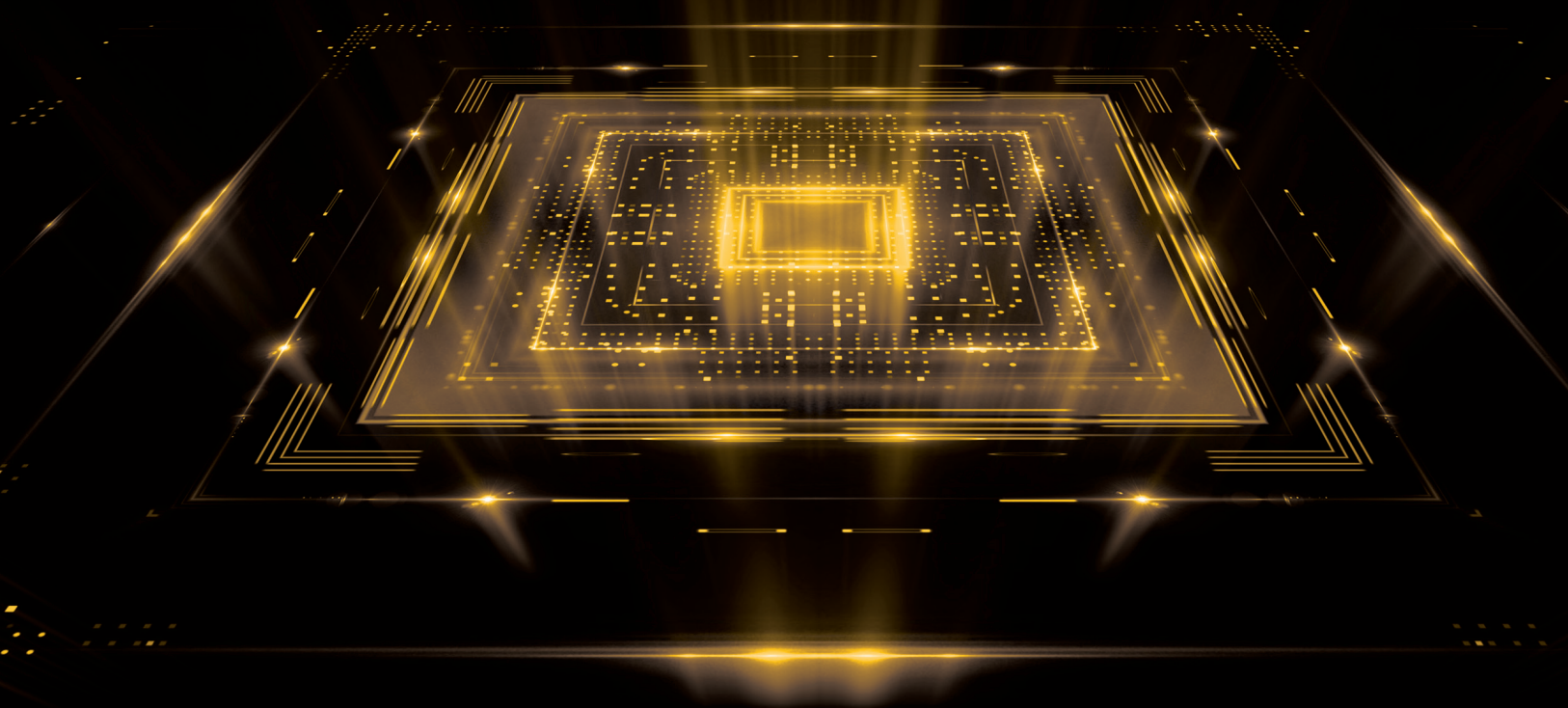
Magazine of the Computing Center of the Slovak Academy of Sciences 2021

hpc focus



EURO SLOVAKIA

Editorial

Dear readers, dear HPC users and enthusiasts,

the HPC Focus magazine is here with a new edition! There have been some changes in the area of high-performance computing in Slovakia since the last issue. Some may have remained unnoticed, some have gained more of a media attention, but we believe that ultimately these changes will bring progress and advancement to our HPC community as a whole.

At the end of April 2021 the SIHPC project has been successfuly concluded. It was thanks to this project that we were able to procure and put into operation the first Slovak supercomputer Aurel in 2012, along with other HPC infrastructure in Bratislava, Žilina, Košicie and Banská Bystrica. Let us acknowledge and say thank you to all of our partners involved in the SIVVP project: the University of Žilina, the Slovak University of Technology in Bratislava, the Technical University of Košice, the Institute of experimental physics of the Slovak Academy of Sciences in Košice, the Institute of Informatics of the Slovak Academy of Sciences in Bratislava and the Matej Bel University in Banská Bystrica. The SIHPC project was a significant step forward in terms of computational performance and capacity in Slovakia and has over 145 project outputs in the form of scientific publications authored by the Slovak HPC users. In compliance with the project terms, only scientific research teams from Slovak public universities and the Slovak Academy od Sciences were granted access to the computational resources.

One of the changes mentioned earlier is the establishment of the National Competence Centre for HPC (NCC) as an institution of first contact for HPC access and services, which will be offered not only to the academic research groups, but to small and medium enterprises, industrial companies and public sector institutions as well.

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The National Competence Centre for HPC is a part a European network of 33 competence centres established as a part of the EuroCC project. Our efforts will be dedicated to awareness creation and the promotion of HPC, as well as strenghtening of competences in the fields of high-performance computing, high-performance data analytics (HPDA), machine learning (ML) and artificial intellience (AI). Among others, our services will include educational courses and workshops, consultations and assistance with the implemetation of HPC solutions and pilot projects.

We feel that opening the Slovak HPC community is an important step in the context of the Digital transformation and transition to the Industry 4.0. Higher uptake of the HPC+ technologies in business and industry, in public sector and science will surely boost the innovation potential in Slovakia.

In recent months, the National Supercomputing Centre (NSCC) was established. As an association of the academic, private and public institutions and organizations, its goal will be to form a much-needed vision and strategies for the development and support of HPC on a national level. Already today, the funding from the Slovak Recovery and Resilience Plan is allocated for building a new supercomputer, which is one of the NSCC goals for the coming years.

Until these ambitious plans and visions are a reality, we are aware of the pressing need to expand and renew the Slovak HPC infrastructure in the short-term. The Centre of Operations, SAS has succeeded with a project proposal for the procurement of the new HPC infrastructure, which will be financed through the Operational Programme Integrated Infrastructure (OPII). We hope to see the new supercomputer in operation early in 2022.

Dear readers, we will strive to implement all of the changes mentioned here in a manner that will bring you even better services and support. We would, of course, appreciate your thoughts and feedback and hope to foster the growing HPC community.

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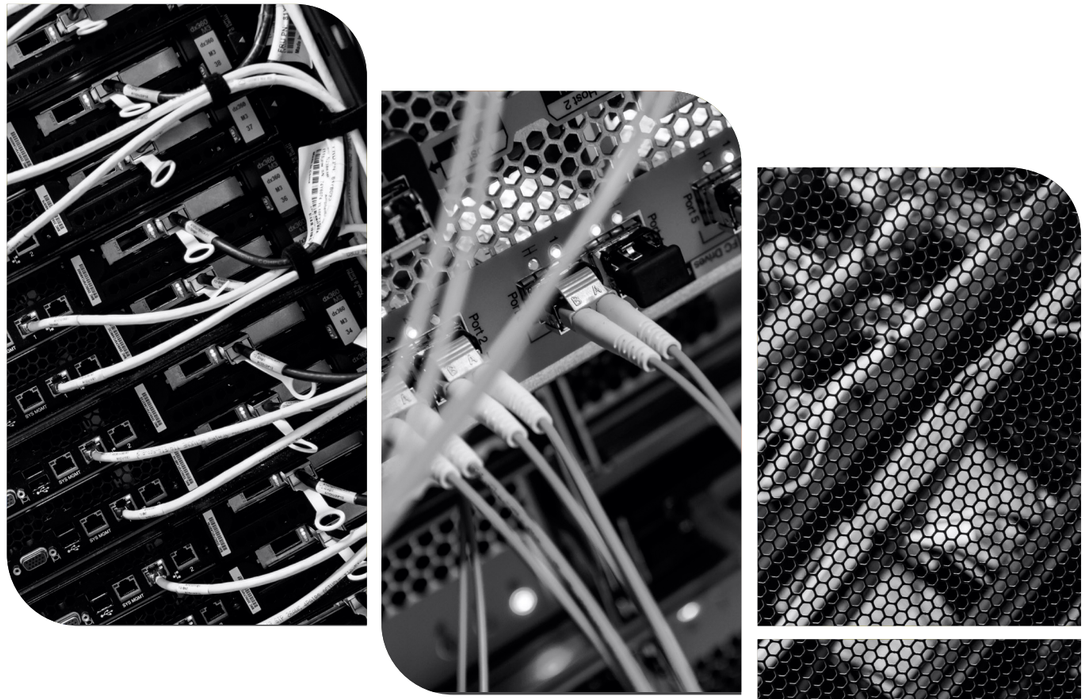

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Podporujeme výskumné aktivity na Slovensku
Projekt je spolufinancovaný zo zdrojov EŠ

01

NSCC
NCC for HPC
EUROHPC

hpc focus

National Supercomputing Center

INTERVIEW WITH LUKÁŠ DEMOVIČ & RADOSLAV REPA

The National Supercomputing Centre (NSCC) was established on November 18, 2020 with the vision to unite and encompass HPC activities in Slovakia. In close cooperation with the National Competence Centre for HPC, it will support education, contribute to the HPC advancement on the national level as well as operate the national HPC infrastructure. State institutions as well as companies from the private sector are members of the NSCC consortium. The Ministry of Investments, Regional Development and Informatization of the Slovak Republic (MIRRI SR), and the Slovak Academy of Sciences (SAS) represent the state sector, while the organization Innovations for Digital Infrastructure (I4DI) represents the private sector. Private companies Towercom, PosAm, IPM group and Tachyum make up the founding members of the I4DI. One of the NSCC's high priority goals is to build a new supercomputer using a unique hardware solution developed by the Tachyum company. The new HPC infrastructure is expected to offer performance on top European level. We talked about the NSCC with members of its administrative board, Radoslav Repa (MIRRI) and Lukáš Demovič (SAS).

The NSCC is a unique combination of public, private and academic sectors. How and when did the idea of establishing a national center dedicated to high-performance computing emerge?

RR: Two years ago, representatives of the Digital Agenda section at today's MIRRI, including me as the Director-General of this section, came up with the idea of connecting all three sectors within a special platform with its own legal subjectivity. In the past, I worked in Brussels on the European digital agenda. Therefore I proposed creating our own entity with members that would bring higher added value to the joint project, each for an area in which they have competencies and skills. Specifically, MIRRI as a partner responsible for the negotiation and implementation of European digital policies, SAS with the Center of Operations of the SAS as a partner responsible for the current operation of the national HPC infrastructure and the I4DI association, including Tachyum with significant innovation potential. The connection of these partners with the established international and domestic contacts and with the clear goal of the implementation of the indicated project of a high performance supercomputer has thus ensured sufficient motivation and direction. Political support for the project is also important, which is guaranteed at the level of the Deputy Prime Minister, as well as by government materials. It should also be mentioned that the triple helix type of connection, where the cooperation of academic, private and public sectors intersects in the field of digital economy development was defined for the first time by the Digital Transformation Strategy of Slovakia 2030 and its action plan. Similar connections have already been established in the field of digital education, artificial intelligence, quantum infrastructure and others.

Lukáš Demovič is the Director of the Centre of the Operations of the SAS and the Chairman of the Administrative Board of the NSCC.

How do you assess the cooperation of these three sectors so far and what are their roles within the NSCC?

RR: I can confirm that the cooperation proceeds in a diligent and professional fashion. When communicating a topic that is highly innovative in the Slovak environment and its application crosses national borders, you will always come across questions about the meaningfulness and justification of the solution for science, for companies, for Slovakia as such. The debates and meetings between partners, which are relatively frequent, do have their own dynamics, but I consider them as positive, as we always manage to find a compromise solution that is advantageous for all parties. Naturally, it happens that the partners also get into an argumentative opposition, as a consequence of their logical setting, when completely different worlds stand against each other, e.g. the public vs. the private sector or even the academy. However, what is essential here is the result, always based on legal certainty, clear rules and a sustainable implementation model. If we manage to define this, I am confident to declare that we will build

a high performance computer. The next step is a feasibility study, giving this ambition an economic raison d'être.

We have a defined and approved an annual work program, which we are implementing. The work on the Recovery and Resilience Plan, as well as the identification and evaluation of the suitability of engaging in international projects for the development of supercomputer infrastructure and capacity building, has so far required the greatest effort. Among other things, it is important to see the NSCC as a liaison point for a wide network of European supercomputing centers, which in itself brings a number of expert challenges and tasks. The human capacity of the NSCC team is still very limited, in accordance with the initial plan to rationalize the operational costs. The professional and managerial capacities of MIRRI, SAS and I4DI were primarily involved in the work itself. Since April, one professional employee in charge of operations has been working for the NSCC, another one will come soon.

LD: I will just add that the NSCC is a newly created legal entity and so it was necessary not only to process all the documents, but mainly to set the internal rules and procedures for the cooperation of all three founding members. And, of course, it takes some time for the partners to learn to speak a common language, because we have a relatively wide range of people with different areas of expertise on the board. However, I think that we have set a very good path and that we have already managed to solve many early problems. Personally, I really like the opportunity of interacting with people from MIRRI, such as Radoslav Repa, Juraj Kubica or Michal Číž, who have an up-to-date overview of planned activities at the national and European level and can define best practices in creating such large-scale projects. I especially appreciate the cooperation in incorporating the topic of the supercomputer into the Recovery and Resilience Plan.

When the NSCC was founded in November 2020, the expectations and a lot of information associated with building a new supercomputer immediately emerged. What are the ambitions of the centre in this regard?

RR: NSCC's primary ambition is to build a high performance supercomputer. We have funds set aside for this purpose from the Recovery and Resilience Plan. Directly managed EU programs, such as the Digital Europe Program, offer other investment opportunities. It directly calls on member states to invest in the construction of supercomputers. Europe has set for itself the goal of creating its own independent computing infrastructure, which has a positive impact on cyber security as well as greater confidence in the digital single market. Our steps will support this goal.

LD: The supercomputer should have the parameters that will rank it among the top in Europe. Whether it is by performance or by the emphasis on the efficiency of its operation or by the possibilities of use for various types of applications. However, we do not currently have suitable premises in Slovakia for such a powerful facility, which is why we want to build it in phases. Each of the planned technologies will be tested so that the machine operation at full power can be achieved as smoothly as possible. In parallel with this process, the construction or upgrade of the data center will be carried out.

What are the goals and plans of the NSCC besides building a supercomputer?

RR: The new high performance supercomputer is, of course, a very crucial topic. In addition to this, the NSCC has in its statutes a number of other tasks, goals and plans covering the supercomputer agenda. The purpose of the association is, for example, the support and development of applications, implementation, research, development of high performance computer systems in the Slovak Republic with regard to the state structural, industrial, technical, regional and social policy.

LD: The supercomputer will be useless without a well-developed environment and user community. Therefore, even before its commissioning, the NSCC „prepares the ground" both by raising awareness of HPC, but also by direct support and consultations with users from academia as well as the private sector. This is possible thanks to the European PRACE and EuroHPC JU projects, in which the Center of Operations of the SAS is involved on behalf of the NSCC. Thanks to these projects, European countries are exchanging experiences, interconnecting their HPC infrastructure, organizing training activities, but also developing applications for future supercomputers. In building relationships with the private sector and the HPC community as such, the NSCC will work closely with the National Competence Center.

Radoslav Repa is the Director General of the Digital Agenda Section. He focuses on the final phase of the implementation of the initiatives of the Digital Single Market Strategy, as well as on the implementation of the newly adopted Strategy for the Digital Transformation of Slovakia until 2030.

NCC for HPC
is
Open for Business

What does it mean for HPC users in Slovakia?

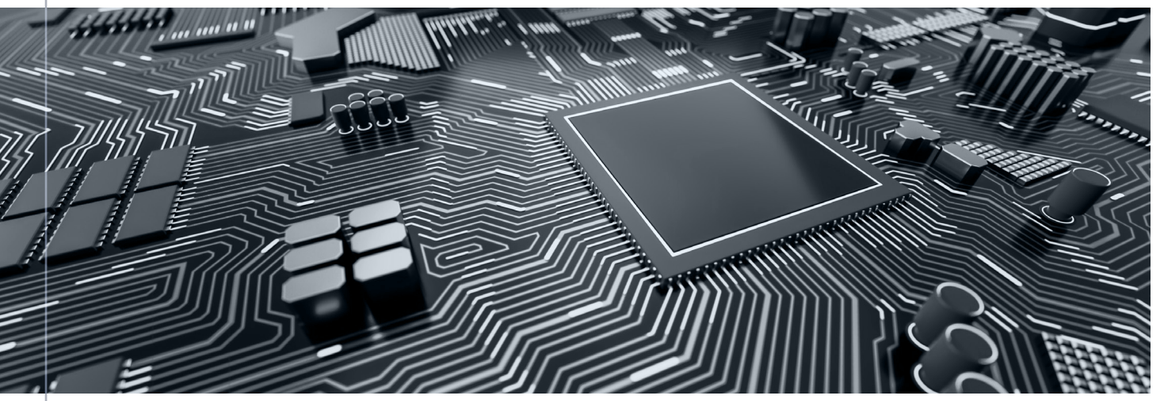
The Centre of Operations of the Slovak Academy of Sciences has joined the EuroCC project, which aims to establish a network of National competence centres across 33 European countries. The project is supported by the EuroHPC JU organization and the implementation is coordinated by the Castiel CSA (Coordination and Support Action). The National competence centres are envisioned as the primary contact points for HPC in any given state, providing services such as education, consultancy and access to resources for users from academia, public administration and the private sector.

The EuroCC project was launched on September 1, 2020 and immediately the COO SAS team started the implementation to secure the operation of the Slovak National Competence Centre for HPC (NCC for HPC). The project duration is two years and during this period the NCC should start fulfilling its mission, which is defined quite broadly: promoting the HPC solutions and tools of high performance data analytics (HPDA), machine learning (ML) and artificial intelligence (AI), providing technical advice and consulting services, educational activities, IT courses and building the HPC community. Being a part of the international network of competence centres, the Slovak NCC can rely on its partners regarding technology and knowledge transfer, and is thus able to provide its clients with services at a European level.

What does this mean for the HPC users in Slovakia? So far, the HPC activities have been covered by the SIHPC project: user registration, project submission, access to computational resources and technical support. These services will be taken over by the NCC for HPC and will be further developed and expanded. We set up our services to correspond with the best practices in Europe as well as with our users' requirements. A new registration portal for HPC users, a new system of project submission and evaluation, as well as other new services for users are being prepared under the auspices of the National Competence Centre.

The National Competence Centre has a website /eurocc.nscc.sk/ with information covering the activities and services it offers. New services include free courses for general public as well as HPC users, currently organized online. One section of the webpage is dedicated to grant and access opportunities for users. PRACE Access, PRACE Shape, PRACE Deci or FF4EuroHPC are among the calls for proposals regularly announced by the PRACE and the EuroHPC JU organizations. In addition to supporting academic research, these schemes also focus on small and medium-sized enterprises, providing access to computing resources in Europe, close cooperation with HPC experts and in some cases also the project funding.

The National Competence Centre is also facilitating access to technical expertise for users via the docs.nscc.sk webpage, where the documentation on computing infrastructure, log-



The National competence centre provides free consultations and guidance and can facilitate contact with European experts.

ging in, job submission, program compilation and running applications can be found all in one place. The plan is also to provide easy-access tools that will simplify and streamline the workload management for HPC users.

Mapping of the HPC+ competencies is another important task for the National competence centre. The goal is to obtain comprehensive information about HPC competencies, the use of HPC solutions and the possibilities of adopting these tools in the Slovak academic, public and private sectors through an online survey. The result - a competence map - will be the starting point for creating strategies for the expansion of the HPC community and further development of cooperation and collaboration in the field. It is likely that the level of knowledge and competence in academia will be comparable to other EU countries, but the uptake of HPC technologies in the public and private sectors is expected to be significantly lower.

Trying to engage and motivate SMEs and industry to adopt the HPC+ tools remains a challenge across Europe. One of the important tasks for the Slovak NCC is therefore the promotion and awareness creation of high performance computing both among potential users and among the general public. By participating in popularization activities and conferences, but also by utilizing the power of social media the competence centre showcases the possibilities of using HPC not only in science, but also in industrial production, research and development.

HPC in Slovakia is perceived mostly as a domain of academia and academic research teams, while the Slovak companies, similarly to those abroad, are facing barriers when adopting these solutions: lack of knowledge and experience, limited access to infrastructure. National competence centres across Europe will help to overcome these barriers, thus implementing the European vision of supporting informatization, digitalization and innovation.

In practice this means that NCC experts will provide free consultations, technical support and facilitate contact with European experts. They will also help to identify optimal solutions, assist with the effective applications setup and with the implementation of pilot or proof-of-concept projects. Currently, the Slovak NCC cooperates with 4 non-academic companies.

In addition to increasing competencies within the HPC community, the Competence Centre ensures continuous education of its own experts. With the support of the Castiel CSA, the EuroCC members participate in trainings and workshops and benefit from intensive exchange of knowledge and experience with other competence centres.

And what about the goals at the national level?

The National Competence Centre, while continuing to provide high quality services and support to all users, will assume the role of the primary contact point for the HPC field in Slovakia and a gateway to the Slovak and European HPC community.

Procurement of the new HPC INFRASTRUCTURE

With the **SIHPC** (Slovak Infrastructure for High-Performance Computing) project nearing its conclusion the Centre of Operations of Slovak Academy of Sciences (CoO SAS) sees the need for an expansion and renewal of the existing HPC infrastructure in Slovakia. During the 2019–2020 period the COO SAS utilized its substantial experience with the operation of HPC systems and taking into account the users requirements, prepared a project proposal within the Operational Program Integrated Infrastructure: OPII-2020/7/55-NP. The project under the name National competence centre for high-performance computing (code 311071AKF2) was successful and its supporting activities commenced in December 2020.

In accordance with the priorities defined by the Slovak Strategy for Digital Transformation, the project aims to support the private sector in Slovakia – small and medium enterprises specifically – and to help raise their innovation potential. This will be achieved by building a platform for effective adoption and utilization of HPC+ technologies. The **EU Structural Funds** will be used for the procurement of a new HPC system, thus providing technical support and basis of the National Competence Centre.

The new HPC system will possess several times higher computational power compared to the currently available infrastructure. Taking into account the growing demand for AI/ML technologies, the system will consist of a typical CPU partition and a partition expanded with general-purpose GPU accelerators. The supercomputer as a whole will be built in a modular fashion (having possible future expansion in mind) utilizing state-of-the-art HPC and network technologies. Of course, a centralized management and system operation monitoring will be a part of the project. Furthermore, the CoO SAS plans to deploy new services, such as ease-of-access tools for the HPC users (OnDemand) and tools for easier utilization of the computational capacities (OpenStack, Singularity,...).

The CoO SAS is working closely with the Ministry of Investments, Regional Development and Informatization of the Slovak Republic, as an intermediary institution, during the implementation of this project. Already the public procurement process has been started at the end of July 2021. The overall project duration, supporting activities included, is 32 months. The new computational capacities are expected to be operational and accessible early in 2022.

EUROHPC JU
PANEUROPEAN HPC INFRASTRUCTURE

The European High Performance Computing Joint Undertaking - EuroHPC JU is a joint inniciative of the European Union, European countries and private sector partners to build a world-class European HPC ecosystem. Slovakia is a member state of the EuroHPC JU since 2019. Today 33 European countries are involved, together with the European Union (represented by the European Commission) and two private partners (ETP4HPC and BDVA).

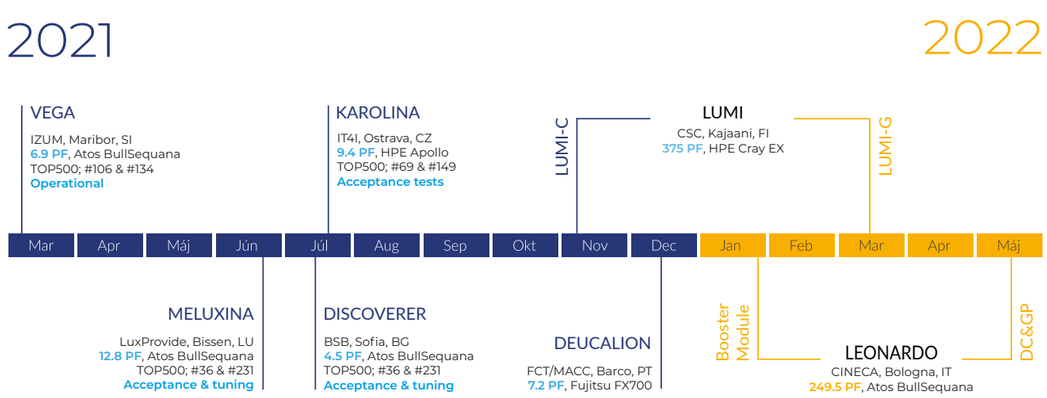
The EuroHPC JU allows the European Union and the EuroHPC JU participating countries to coordinate their efforts and pool their resources to make Europe a world leader in supercomputing. This will boost Europe's scientific excellence and industrial strength; support the digital transformation of its economy while ensuring its technological sovereignty.

From the user's point of view the information about new European supercomputers is the most interesting, since the EuroHPC JU offers possibilities of access to academic and private users. At the moment seven out of eight planned projects are in the process of either procurement or installation (five petascale, three pre-exascale) and should be in operation in May 2022:

The following pages provide Overview and details of the European HPC systems.

EUROHPC SYSTEMS ROLLOUT SCHEDULE

EuroHPC Joint Undertaking



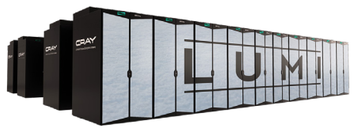


Illustration of the HPE Cray EX cabinets
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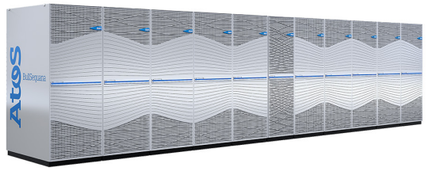

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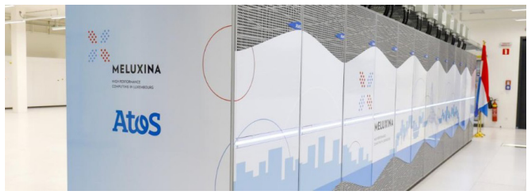


	LUMI	LEONARDO
TECHNOLOGY	The LUMI system will be a Cray EX supercomputer supplied by Hewlett Packard Enterprise (HPE) and located in Finland.	Leonardo will be supplied by ATOS, based on a BullSequana XH2000 supercomputer and located in Italy (Tecnopolo di Bologna).
SUSTAINED PERFORMANCE	375 petaflops	249,4 petaflops
PEAK PERFORMANCE	552 petaflops	322,6 petaflops
COMPUTE PARTITIONS	▸ GPU partition (LUMI-G) ▸ 86 CPU-partition (LUMI-C) ▸ data analytics partition (LUMI-D) ▸ container cloud partition (LUMI-K)	▸ Booster, hybrid CPU-GPU module delivering 240 Pflops ▸ Data-Centric, delivering 9 Pflops and featuring DDR5 Memory and local NVM for data analysis
CENTRAL PROCESSING UNIT (CPU)	The LUMI-C partition will feature 64-core next-generation AMD EPYC™ CPUs	Intel Ice-Lake (Booster), Intel Sapphire Rapids (data-centric)
GRAPHICS PROCESSING UNIT (GPU)	LUMI-G based on the future generation AMD Instinct™ GPU	NVIDIA Ampere architecture-based GPUs, delivering 10 exaflops of FP16 Tensor Flow AI performance
STORAGE CAPACITY	In total, LUMI will have a storage of 117 petabytes and a maximum I/O bandwidth of 2 terabytes per second.	Leonardo is equipped with over 100 petabytes of state-of-the-art storage capacity and 5 PB of High Performance storage.
APPLICATIONS	AI, especially deep learning, and traditional large scale simulations combined with massive scale data analytics in solving one research problem.	The system targets: modular computing, scalable computing applications, data-analysis computing applications, visualization applications and interactive computing applications, urgent and cloud computing.

	MELUXINA	VEGA
TECHNOLOGY	MeluXina will be supplied by Atos, based on the BullSequana XH2000 supercomputer platform and located in Luxembourg.	Vega was supplied by Atos, based on the BullSequana XH2000 supercomputer and located in Slovenia.
SUSTAINED PERFORMANCE	Committed 10 petaflops HPL (Accelerator – GPU Module), 2+ petaflops HPL (Cluster Module)	6,9 petaflops
PEAK PERFORMANCE	Expected 15+ petaflops HPL and ~500 petaflops AI (Accelerator - GPU Module), 3+ petaflops HPL (Cluster Module)	10,1 petaflops
COMPUTE PARTITIONS	▸ Cluster ▸ Accelerator – GPU ▸ Accelerator – FPGA ▸ Large Memory	▸ CPU partition: 960 nodes, 256 GB memory/ node, 20% double memory, HDR100 ▸ GPU partition: 60 nodes, HDR200
CENTRAL PROCESSING UNIT (CPU)	AMD EPYC	122.800 cores, 1920 CPUs, AMD Epyc 7H12
GRAPHICS PROCESSING UNIT (GPU)	NVIDIA Ampere A100	240 Nvidia A100 cards
STORAGE CAPACITY	20 petabytes main storage with an all-flash scratch tier at 400 GB/s, and a 5 petabytes tape library expandable to 100 petabytes	High-performance NVMe Lustre (1PB), large-capacity Ceph (23PB)
APPLICATIONS	Traditional Computational, AI and Big Data/HPDA workloads	Traditional Computational, AI, Big Data/HPDA, Large-scale data processing

© Fujitsu

	KAROLINA	DISCOVERER	DECAULION
TECHNOLOGY	Karolina is supplied by Hewlett Packard Enterprise (HPE), based on an HPE Apollo 2000Gen10 Plus and HPE Apollo 6500 supercomputers and located in the Czech Republic.	Discoverer will be supplied by Atos, based on a BullSequana XH2000 supercomputer and located in Bulgaria.	Deucalion supercomputer will be supplied by Fujitsu and located in Portugal. It will combine a Fujitsu PRIMEHPC (ARM partition) and Atos Bull Sequana (x86 partitions).
SUSTAINED PERFORMANCE	9,13 petaflops	4,44 petaflops	7,22 petaflops
PEAK PERFORMANCE	15,2 petaflops	6 petaflops	10 petaflops
COMPUTE PARTITIONS	▸ a universal part for standard numerical simulations / 720 computer servers / 3.8 PFlop/s ▸ an accelerated part /70 servers / 8 GPU accelerators (11 PFlop/s for standard HPC simulations and up to 150 PFlop/s for AI ▸ a part designated for large dataset processing /24 TB memory / 74 TFlop/s ▸ loud services: 36 servers / 131 TFlop/s	▸ One partition providing 1128 nodes, 4,44 petaflops	▸ ARM Partition: 1632 nodes, 3.8 PFLops ▸ x86 Partition: 500 nodes, 1,62 PFLops ▸ Accelerated: 33 nodes, 1,72 PFLops
CENTRAL PROCESSING UNIT (CPU)	More than 100,000 CPU cores and 250 TB of RAM	AMD EPYC 7H12 64core, 2.6 GHz, 280 W (Code name Rome)	A64FX (ARM partition), AMD EPYC (x86 partitions)
GRAPHICS PROCESSING UNIT (GPU)	More than 3.8 million CUDA cores / 240,000 tensor cores of NVIDIA A100 Tensor Core GPU accelerators with a total of 22.4 TB of superfast HBM2 memory		NVidia Ampere
STORAGE CAPACITY	More than 1 petabyte of user data with high-speed data storage with a speed of 1 TB/s	2 petabytes	430 TB High-speed NVMe partition, 10.6 PB high-speed based Parallel File System partition.
APPLICATIONS	Traditional Computational, AI, Big Data	Traditional Computational	Traditional Computational, AI, Big Data

Access to computational resources and the opportunity to run calculations on the HPC systems built in collaboration with the EuroHPC JU will be open to all European users from academia and industry. The access modes are based on those of the PRACE-RI organization and will be based on several parameters, such as the volume of resources, complexity of the project evaluation, type and complexity of applications and the periodicity of cut-off dates. Specific details will be published together with the respective call for proposals, but a general overview can be seen in the table.

Access to computational resources and the opportunity to run calculations on the HPC systems built in collaboration with the EuroHPC JU will be open to all European users from academia and industry.

A call for a given access mode will typically offer access to several systems. This provides both economy of scale in processing the calls and room for maximizing the volume of allocation. Six Access Modes are taken into consideration for EuroHPC:

- Extreme Scale Access
- Regular Access
- Benchmark Access
- Development Access
- Fast Track Access for Academia
- Fast Track Access for Industry

We publish details about various access calls via the National Competence Centre webpage and send out the information to our Newsletterr subscribers.

ACCESS CATEGORIES

CALL	EXTREME SCALE	REGULAR	BENCHMARK	DEVELOPMENT	FAST TRACK ACADEMIA	FAST TRACK INDUSTRY
DURATION	1 year renewable	1 year renewable	2 – 3 mesiace	1 year renewable	< 6 months	1 year renewable
PERIODICITY	Continuous call, bi-yearly cut-offs	Continuous call, cut-offs every four months	Continuous call, monthly cut-offs	Continuous call, monthly cut-offs	Continuous call, cut-offs ev. 2 weeks /1 month	Continuous call, cut-offs ev. 2 weeks /1 month
DATA STORAGE	Large storage for medium to long term	Large storage for medium to long term	Limited	Data processing environment and platform		
ACCESSIBLE FOR INDUSTRY?	Yes –Open R&D, With specific evaluation criteria	Yes –Open R&D, With specific track	Yes – Open R&D	Yes – Open R&D	No – use industry Fast Track instead	Exclusively Open R&D
APPLICATION						
EXTERNAL PEER-REVIEW EVALUATION	Yes	Yes	No	No	No / Pre-identified	No / Pre-identified
TECHNICAL ASSESSMENT	Yes	Yes	Yes	Yes	Yes	Yes
APPLICATION TYPE	Full application	Full application	Technical application	Technical application	Light request + support documents	Full application
DATA MANAGEMENT PLAN	Yes	Yes	Yes	Yes	Yes	Yes
PREREQUISITES	Benchmark	Benchmark	None	None	Previous allocation or Benchmark	Benchmark
SUBMISSION PERIOD	> 2 months	> 2 months	N/A	N/A	N/A	N/A
EVALUATION PROCESS	3 months	2 months	Up to 2 weeks	Up to 2 weeks	Up to 1 month	Up to 1 month

Small and medium enterprises and industrial companies can apply in all of these categories and access modes or opt for commercial access offered by the EuroHPC JU. The commercial access is offered for civilian applications only.

02

HPC Applications

hpc focus

THE GROUP OF
Prof. Ivan Štich

SUPERCOMPUTER MODELING AT THE NANOSCALE

Prof. Ivan Štich is scientific researcher at the Institute of Physics of the Slovak Academy of Sciences.

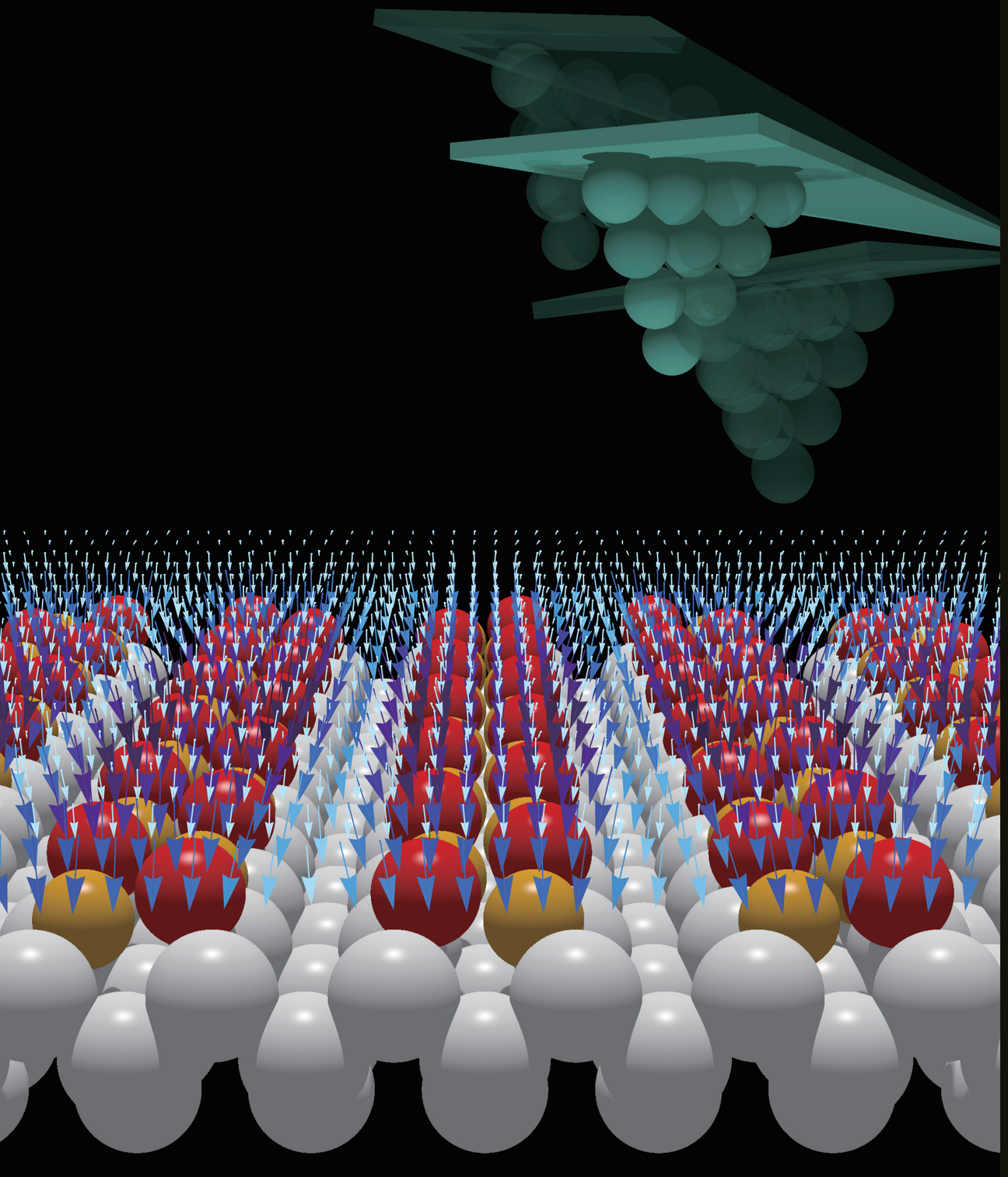
The group of Prof. Štich (Prof. Ivan Štich, Dr. Ján Brndiar, Dr. Róbert Turanský, Dr. Kamil Tokár, and until May 2018 also Dr. René Derian) at the Institute of Physics of the Slovak Academy of Sciences has a long-term interest in supercomputer atomic-scale modeling of condensed matter systems (3D crystals, surfaces, 2D systems, molecules). Behavior of matter at the atomic-scale is governed by quantum mechanics, i.e. by the Schrödinger or Dirac equations. Supercomputer modeling typically solves those equations numerically for systems comprised of hundreds of atoms and hundreds to thousands of electrons. Such calculations are usually computationally very demanding. As an example, to determine the band gap of 2D phosphorene using the ultra-accurate stochastic quantum Monte Carlo methods, see below, which, if run on the Slovak supercomputer Aurel, would require roughly its full one year capacity. In the last few years the group of Prof. Štich has used the modeling primarily as a tool for interpretation or verification of laboratory experiments in close collaboration with European partners such as Regensburg University, Giessen University, and laboratories in Japan, in particular with Osaka University and with North Carolina State University in the USA. We will briefly introduce a few examples of the modeling results below.

Photo of the CCMS group at the IP SAS: prof. Štich, Dr. Brndiar, Dr. Turanský, Dr. Derian & Dr. Tokár.

01 Collaboration with Prof. Sugawar and Prof. Li

The Osaka University, Japan

With the Sugawara-Li group at the Osaka University we have a collaborative project on non-contact atomic force microscopy (AFM). AFM is an experimental method which makes it possible to image surfaces of solids with atomic, in rare cases with subatomic resolution, nanomanipulation of atoms and molecules on surfaces, and which in some cases exhibits also chemical resolution, i.e. makes it possible to determine the type of atom under the tip of the microscope. All these abilities are derived from the force acting between the tip and the sample. Numerical simulations of the AFM experiments usually enable to determine the apex of the tip, i.e. of the atom terminating the tip which is mapping the surface underneath with atomic resolution or the tip-sample distance which is also unknown from experiments only.



In 2017 we have, in collaboration with our Osaka partner, for the first time shown how vector quantities can be measured with AFM methods, example being for instance the forces acting between the AFM tip and sample, dipole moments or magnetic moments which all were approximated by the z-component of the vector quantity. An example being the force vector field measured above the dimers of the germanium Ge(001)c(4 × 2) surface in ultra-high vacuum at liquid nitrogen temperatures, see the figure on the right [1]. We have numerically modeled this force map and found that the forces computed from our model are one order of magnitude larger than those measured experimentally. Explanation of such a discrepancy by failure of our model was not possible. Therefore a new analysis of the experimental data and their conversion to the force vector map was performed. As a result we detected an error in the experimental data conversion which led to the experimental estimate of the tip-sample distance by approximately 1 Å (1 Å = 10^{-10}m). After applying that correction the agreement between the experimental and simulation data was almost quantitative. Another consequence of the discrepancy we found was that we have proposed a novel method which makes it for the first time possible to determine the tip apex-sample distance directly from the measured vector force map. In a wider context we anticipate that atomic-scale knowledge of the distribution of forces above a surface, both lateral and vertical, will open up a new window on understanding the morphology of surfaces, their chemical composition and the surface chemical reactions, study of nanostructures via atomic and molecular manipulation and understanding of behavior of nano-machines on surfaces.

02 Collaboration with the group of Prof. Schirmeisen

University Giessen, Germany

Another example of how numerical simulations can aid understanding and interpretation of laboratory experiments, this time AFM in the so-called contact mode, is our nanotribology project, i.e. nano-scale friction, a collaborative project with the research group of Prof. Schirmeisen, University Giessen, Germany. At variance with the macroworld

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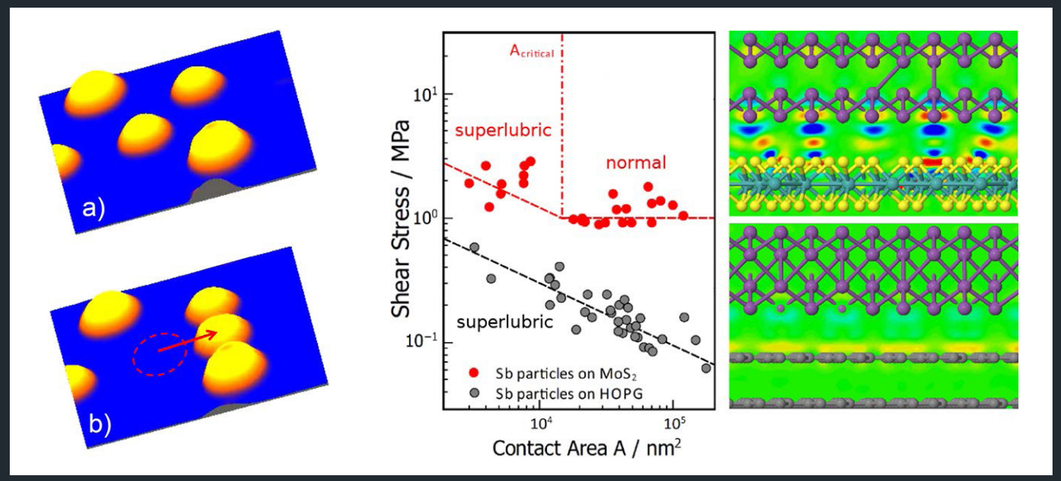
where surfaces in contact always exhibit some friction, the surfaces at the nano-scale, under certain circumstances, can realize a state where surfaces can translate without any measurable friction and exhibit the so-called superlubricity. In simple terms, the theory of superlubricity explains the finding by incommensurable surfaces which, due to different lattice constants of the nanoparticle and substrate or due to incommensurable orientation of the nanoparticle and substrate do not "fall into registry". As most combinations of materials exhibit different lattice constants the superlubricity should be commonplace which contradicts the reality.



For understanding the conditions in the nano-world necessary for realization of the superlubric state we have compared friction of relatively massive antimony nanoparticles on graphite (HOPG) and MoS2 in ultra-high vacuum [2]. Note that both surfaces are quite similar and well-known lubricants. The results in the figure above show that the two systems indeed exhibit completely different tribological properties. As the figure proves all antimony nanoparticles on HOPG are superlubric, whereas on MoS2 only smaller nanoparticles exhibit superlubric behavior and the larger ones exhibit normal friction. We have shown that such a behavior is due to emission of dislocations on the Sb/MoS2 nanocontact absent from the Sb/HOPG. As a result, the Sb/MoS2 nanocontact is locally „in registry" for larger nanoparticles and Sb/HOPG is not. In addition, as the calculated charge densities shown in the figure above show, the two nanocontacts have completely different chemical properties which also contribute to a higher degree of friction on the Sb/MoS2 compared to Sb/HOPG nanocontact.

Our study was the first demonstration of the influence of the nanocontacts on tribological properties at the nanoscale. It is evident that similar conditions for superlubricity appearance will also be valid in other systems, which is the reason why superlubricity is more an extraordinary than usual behavior. It is also evident that a thorough understanding of superlubricity at the nanoscale is a necessary condition for a practical exploration of this phenomenon.

03 Collaboration with Prof. Fabian and Prof. Mitas

University Regensburg
North Carolina State Univerzity

The third example from our current research is related to electronic and photonic properties of 2D materials. After Nobel prize awarded in 2010 to Geim and Novoselov for discovery of unique properties of graphene (a 2D analogue of graphite), 2D materials are currently of the hottest topics in materials science. While electronic properties of 2D materials cover metallic layers of palladium and rhodium, semimetallic graphene, semiconductors with different bandgaps, such as silicone, phosphorene and transition metal dichalcogenides, and wide-bandgap h-BN, perhaps the most important 2D materials are those which feature a bandgap. Bandgaps, the key parameters for electronic applications, can further be tuned by the number of layers, strain, chemical doping, dielectric embedding (substrate and capping), etc. However, it turns out that an accurate measuring of the bandgaps in 2D materials is a technical problem. For instance, for single-layer phosphorene, a direct bandgap material, photoluminescence spectra yield optical bandgaps between 1.3 and 2.1 eV, i.e. with unacceptable scatter of ≈ 0.8 eV. Such a scatter cover spectrum from infrared to green light! The scientists and engineers would certainly like to know if phosphorene could be used as a material for LEDs emitting red, yellow, green or blue light. Similar bandgap scatter is also found in other 2D materials. In such a situation, one could expect that the reference

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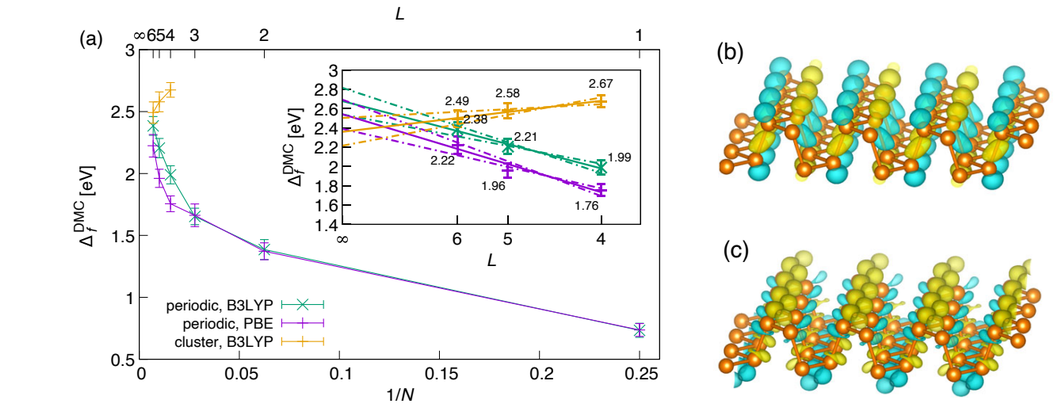
bandgap value could simply be determined by calculation. Sadly, it turns out that similarly to experiments the numerical methods (DFT, or GW) too exhibit a similar scatter. Therefore we have set up a collaborative project with Prof. Fabian, University Regensburg, and Prof. Mitas, North Carolina State University, on modeling bandgaps via stochastic many-body quantum Monte Carlo methods [3].



The quantum Monte Carlo methods are among the most accurate electronic structure methods and represent a completely different computational paradigm. We calculated the bandgap from the difference of the many-body energies of ground state (HOMO, panel b) in the figure above) and first excited state (LUMO panel c). The results are summarized in the figure above which shows finite-size scaling to thermodynamic limit (limit of an infinite system). From that figure it is also evident that for a sufficiently large system the scaling is linear in 1/N, where N is the number of atoms or electrons in the system. The calculation was done for both cluster (yellow color) and periodic approximants (pink and green color, which correspond to two different preparations of the so-called nodal hypersurfaces, i.e. surfaces where the wavefunction is zero). The extrapolated bandgap (so-called quasi-particle gap) determined is ≈ 2.4 eV (or the estimated optical bandgap is ≈ 1.75 eV), i.e. at the upper limit of the experimental values. These extrapolated values of the bandgap are likely the most accurate estimates of a bandgap in a 2D material and represent a unique case where a calculated value is likely more accurate than the experimental one. The flip-side of the coin is the cost of the energies in the above figure. We needed about 30 million core hours to calculate them, which is an equivalent of one full year capacity of the Slovak supercomputer Aurel and shows that the cost of knowledge is always high. This cost is payed off by ultimate knowledge, understanding, and shining light onto the experimental and theoretical accuracies. We are currently applying this computational model to other 2D materials and to 2D materials under applied strain.

We needed about 30 million core hours to calculate the energies in the figure on the left, which is an equivalent of one full year capacity of the Slovak supercomputer Aurel and shows that the cost of knowledge is always high.

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[2] D. Dietzel, J. Brndiar, I. Štich, and A. Schirmeisen. *Limitations of Structural Superlubricity: Chemical Bonds versus Contact Size*, ACS Nano 11, 7642 (2017).

[3] T. Frank, R. Derian, K. Tokar, L. Mitas, J. Fabian, I. Štich. *Many-body quantum Monte Carlo study of 2D materials: cohesion and band gap in single-layer phosphorene*, Phys. Rev. X 9, 011018 (2019).

THE COST OF COMPUTING TIME ON A SUPERCOMPUTER IS BALANCED BY THE ULTIMATE KNOWLEDGE AND UNDERSTANDING.

FUNCTIONAL CLAYS & HPC

Eva Scholtzová

Clays are present all around us. People have been using this functional material in everyday life since ancient times. We often ignore them, failing to recognize their omnipresence and practicality. For example, cosmetics, toothpaste, cleaning and washing powders, ceramics – whether it is cups, plates, sanitation, or bricks and tiles, paved sidewalks, as well as high-quality paper and bleaching clays for mineral oils, all contain clays. They also have the use in other fields of industry such as construction, chemistry (catalysts, fertilizer carriers, paint fillers, radiation-resistant materials and absorption agents). The quality of soils is also influenced by the presence of clays, which specify their correct usage.

In recent times, clays were categorized among substances directly protecting the environment. With their ability to swell and hydrate together with the binding of the organic matter in the interlayer space, clays are able to degrade and immobilize toxic materials as well as prevent the spreading of undesirable substances in the environment (waste dumps). Clay minerals, e.g., montmorillonite, or kaolinite, as well as clay-based hybrid materials are becoming very popular in the industrial applications and development of advanced materials with precisely defined physicochemical properties. They are known for their layered structure with mutually connected sheets of tetrahedra (T) and octahedra (O) into layers, either in T-O or T-O-T formations. In the interlayer space, clay minerals contain inorganic cations, quite often hydrated, that balance the charge of the layers caused by the isomorphic substitution of central cations in the polyhedra of the individual layers. These inorganic cations (e.g., Na^+, Ca^+) can be replaced by organic molecules/cations that are usually present in the soil or wastewater (e.g., pesticides, pharmaceuticals, heavy metal cations, etc.) and hold them in their structure using the so-called cation exchange reaction (Fig. 1). The ability of clays to swell is also used for the preparation of organoclays with specific properties, where a small organic cation can be replaced by larger organic cations. Therefore, it is also very important to study the stability of these hybrid materials.

Dr. Eva Scholtzová is a scientific researcher in the Department of Theoretical Chemistry at the Institute of Inorganic Chemistry SAS.

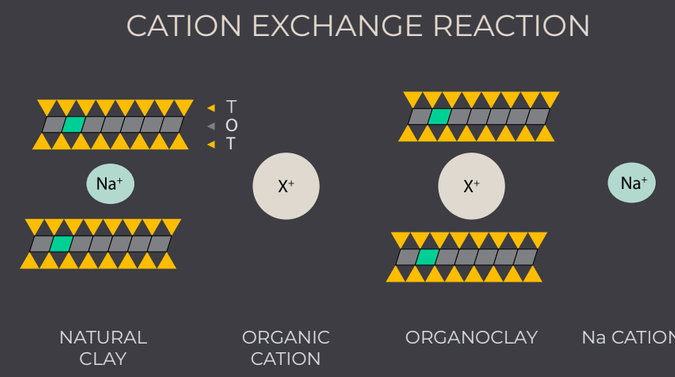

FIGURE 1

Schematic illustration of the structure of Na-montmorillonite (T-O-T type of structure) and the formation of the organoclay by the exchange of an inorganic cation for an organic one.

Conventional research and development of new hybrid materials (organoclays) is usually a very lengthy and financially demanding process. The new material needs to be synthesized (very often the use of the expensive chemicals harmful to health requiring special manipulation) and then its physicochemical properties need to be tested using var-

ious experimental techniques (expensive measurement time, instruments accessibility, etc.). In spite of precise synthesis and rigorous testing, the new material might not satisfy our expectations based on predefined requirements. A large amount of material, energy and finances can be saved by using the techniques of theoretical chemistry and employing the HPC.

Thanks to the enormous progress in the HPC and the development of new theoretical methods the use of which is now common practice, it can be designed more sophisticated and more realistic models of the solid state and thus also of hybrid materials. Using models with hundreds and even thousands of atoms allows us to simulate the structure of the new material and study its physicochemical properties. The number of practical experiments can be significantly reduced, and the design of a material with desired properties can be much faster and more effective.

For example, it is very desirable to know the progress of the intercalation of clay materials during the preparation of organoclays. Models calculated using quantum chemical methods such as *ab initio* DTF (Density Functional Theory) method, provide effective answers to questions concerning the process of binding organic substances in the interlayer space of clay minerals, the stability of organoclays, and their mechanical and spectral properties. Measured infrared, Raman as well as UV/VIS spectra, are usually very complex for these substances, thus the identification of the individual bands very difficult, if not impossible (for example, due to bands overlapping). Structural models and calculations are very helpful here. Detailed analysis of calculated vibrational modes of the individual functional groups can accurately describe not only the bands in the spectrum but also clarify more subtle effects, e.g., red/blue shift of CH vibration bands in the infrared spectra. Computational models need to be sufficiently sized to show the required properties and phenomena. The size of the model also increases its computational demand and brings the necessity of using HPC tools. Parallel computing is the only way to reach reasonable results for these models in real time (ca. 500 atoms).

Due to their aforementioned effectiveness, I pursue applying computational methods to the structure of clay minerals as well as hybrid materials based on them. For example, it was possible to describe the mechanical properties of grafted kaolinite by methoxy group, which showed, that it is a perspective material for the preparation of polymer nanocomposites, employing parallel computing on the Aurel supercomputer. The methoxy group present in the structure of kaolinite improves the exfoliating properties of the kaolinite layers dispersing thus this organoclay (methoxy-kaolinite, Fig. 2a) more easily in a polymer matrix than the unmodified kaolinite. The analysis of the calculated vibrational modes and its comparison with the experimentally measured spectra revealed that the synthesized hybrid material contained in the interlayer space of kaolinite not only a grafted methoxy group but also some intercalated methanol and water molecules (Fig. 2b), probably due to the abundance of methanol during the synthesis of the organoclay and water being commonly present in the majority of clay minerals. Calculations have shown that their presence actually increases the exfoliation properties of the grafted kaolinitwe (ca. + 15%).

HPC deployment enabled to achieve interesting results for better characterization of the prepared material, revealing its properties desirable for the synthesis of new polymer nanocomposites.

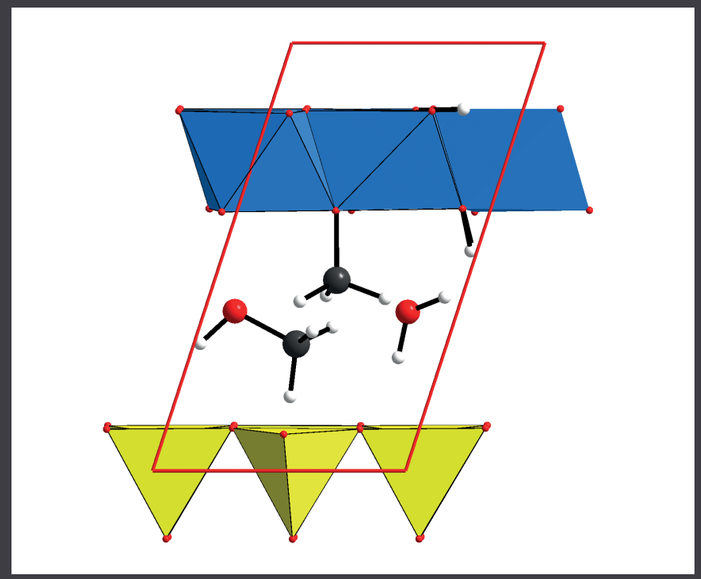

FIGURE 2A

Structural model of the grafted kaolinite by the methoxy group with intercalated molecules of methanol and water in the interlayer space (K-MIXW). Blue – octahedral sheet, yellow – tetrahedral sheet, red – oxygen, black – carbon, white – hydrogen, *a view*.

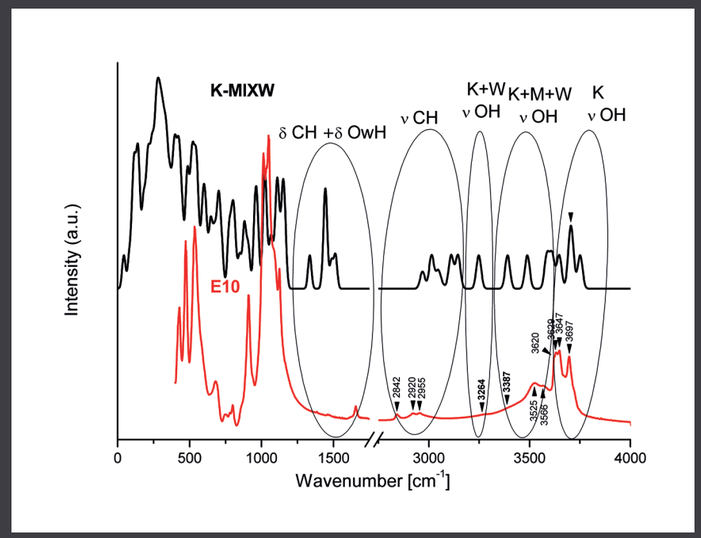

FIGURE 2B

Calculated (black – K-MIXW) and experimentally measured FTIR spectrum (red – E10 sample) of the grafted kaolinite by the methoxy group.

Legend: K-MIXW – grafted kaolinite by the methoxy group with methanol and water in the interlayer space, K – kaolinite, M – methanol, W – water, OH – hydroxy group, CH – CH3 group, ν – valence and δ – deformation vibration.

ACKNOWLEDGMENTS

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Three-dimensional structure of saccharides and their intermolecular complexes with proteins

MILOŠ HRICOVÍNI

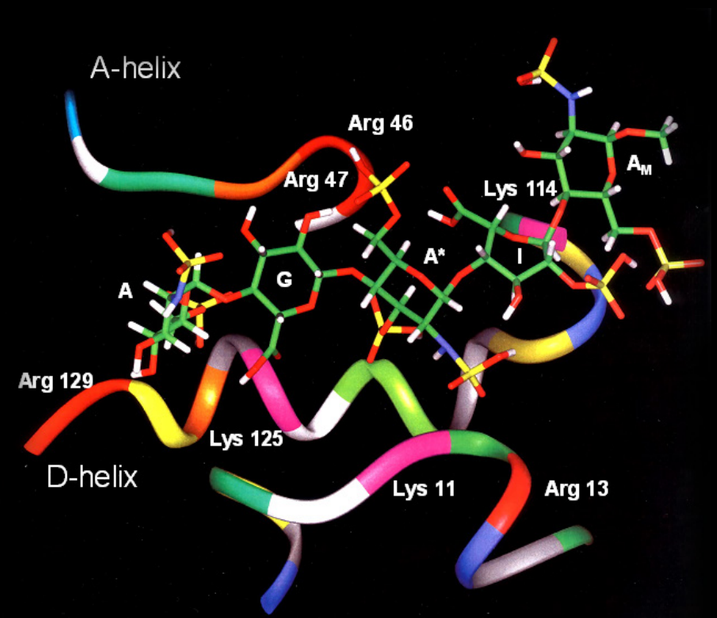


FIGURE 1

Structure of heparin–pentasaccharide–antithrombin III complex.

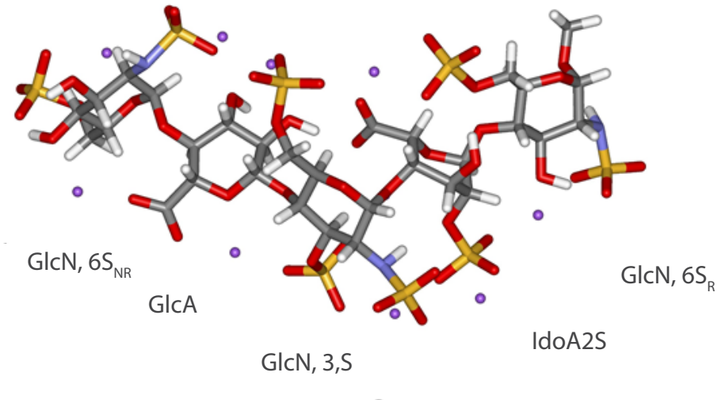
Dr. Miloš Hricovíni is the Head of the Department of Structure and Function of Saccharides at the Institute of Chemistry SAS.

Saccharides and their conjugates belong to essential biomolecules of life. Although sucrose (comprising from two monosaccharides – glucose and fructose) and cellulose (linear polysaccharide consisting of glucose) belong to the most well-known carbohydrates, current interests of chemists and biochemists are focused on saccharides that could be applied in medicinal chemistry due to their biological properties.

The variety of biological properties of saccharides is remarkably large – apart from their known roles as the energy sources in living systems, they have important functions in various processes, such as cell growth and differentiation, angiogenesis, blood coagulation, inflammatory processes, etc. The mentioned large variety of different properties originates from the carbohydrate structural diversity. Carbohydrates can exist as relatively small molecules – mono- or disaccharides, they can form the mentioned linear polymeric forms, but also very complex branched structures or conjugates with other type of molecules, such as proteins or lipids. The knowledge of carbohydrate structures, their solution dynamics and formation of intermolecular complexes is a prerequisite for the understanding of the saccharide functions in biological systems. Apart from experimental techniques (mainly high-resolution NMR at present), computational chemistry methods are essential in biomolecular structure analysis.

One of the mostly studied carbohydrate derivatives are glycosaminoglycans, e.g. heparin, chondroitin sulphate or hyaluronic acid. The anticoagulant properties of polysaccharide heparin were discovered about a hundred years ago and this polysaccharide has been using in medicinal practice since about 1930. The analysis of its structure took quite a long time and the details on the mechanisms of its action was fully understood only recently. Heparin is a heterogeneous polymer, made up from alternating uronic acid (iduronic – IdoA or glucuronic – GlcA) and glucosamine units (GlcN), and most of these units are sulphated in various positions. Heparin molecule specifically binds to protein antithrombin III initiating a cascade of processes that lead to changes of blood coagulation. The structure of the binding sites of both heparin (i.e. part of the polysaccharide that binds to protein) and antithrombin had to be determined in order to understand all details of this protein–carbohydrate interaction. It was soon evident that only about every third polymer chain has a unique sequence of five differently substituted pyranose units – three GlcN (2 x di- and 1 x tri-substituted), one IdoA (monosulphated) and one GlcA (non-sulphated) (Fig. 2). This pentasaccharide binds to the antithrombin binding site (Fig. 1). NMR experiments and theoretical analysis showed that the sulphate groups at the pyranose rings interact with amino acids in the binding site, namely Arg129, Lys125, Lys11, Lys114, Arg13, Arg46 and Arg47. For example, the 6-SO_3- group in the GlcN6S unit interacts with two NH_2 groups in Arg129 and

FIGURE 2



Structure of heparin–pentasaccharide (methyl glycoside) obtained by the geometry optimisation using the DFT method on Aurel supercomputer. Sequence of five saccharide units represents the binding site of polysaccharide heparin with protein antithrombin III. IdoA unit is in the $^{1}C_{4}$ form (upper part, a) or in the $^{2}S_{0}$ form (b). Violet dots represent sodium ions.

in Lys125, other important interactions are between Lys125 and carboxylate in GlcA, as well as among the N-SO_3- group with Arg13 and Lys114. All mentioned amino acids interact with the negatively charged groups in heparin, except of the 2-SO_3- group in IdoA. The role of this sulpho group is indirect, i.e. this group just influences the three dimensional structure of the pentasaccharide during the interaction with the protein. DFT calculations performed on the Aurel supercomputer showed that the conformational equilibrium of the IdoA unit is shifted (with respect to the non-substituted form) from the $^{1}C_{4}$ form (Fig. 2a) towards the $^{2}S_{0}$ form (Fig. 2b) due to the presence of the 2-SO_3- group in solution (the ratio is about 15:85). The $^{2}S_{0}$ form is stabilized in the presence of the protein, i.e. only this conformation is present at the binding site. The presence of the 2-SO_3- group in IdoA affects the spatial arrangement of the reducing end of the GlcN residue and results in the formation of a three-dimensional structure of the ligand (pentasaccharide) that enables the interaction of the N-sulfo group with Arg46, Arg47 and Lys114 in the protein–pentasaccharide complex. When the IdoA residue is not substituted, the solution conformation is significantly shifted towards the $^{1}C_{4}$ form and the energy required for the formation of the protein–saccharide complex is much higher leading to the decreased pentasacharide activity (by about two orders).

The presented heparin–pentasaccharide–antithrombin interaction, as well as other interactions between heparin oligosaccharides (tetrasaccharides, hexasaccharides) with various proteins (e.g. growth factors), belongs to very specific intermolecular interactions. Analyses of the three-dimensional structure of saccharides, proteins, and their intermolecular complexes, by theoretical methods contribute to the understanding of many important biochemical processes in living systems.

Analyses of the 3D structure of saccharides, proteins, and their intermolecular complexes, by theoretical methods contribute to the understanding of many important biochemical processes in living systems.

HIGH PERFORMANCE COMPUTING AND WEATHER FORECASTING AT SHMU

JOZEF VIVODA
MARTIN BELLUŠ
MÁRIA DERKOVÁ

Jozef Vivoda is currently working in the field of NWP at SHMU. He is engaged in atmospheric dynamics model research. Most recent publication: "Finite elements used in vertical discretization of fully compressible core of the ALADIN system."

Weather forecasting using numerical methods for solving equations describing atmospheric motions on high-performance computing (HPC) systems is known as numerical weather prediction (NWP). It is an applied scientific discipline that was founded together with the first ENIAC computer in 1950 in the US. Upon the initiative of J. von Neumann, J. Charney produced the first successful weather forecast based on the barotropic vorticity equation. The first operational deployment of numerical weather forecasts was carried out in 1954 in Sweden and then a few months later in the US. Slovakia had to wait for the first operational numerical weather forecast until the 1st of July 2004. At that time, the operational NWP utilizing model ALADIN on the high-performance computing system at SHMU was launched. The HPC system was delivered in January of the same year. It was an IBM Regatta p690 with 32 POWER4 CPUs and 32 GB of memory. This allowed us to start with the operational weather prediction on a horizontal grid of 9 km x 9 km with 37 vertical levels.

The delivery of IBM technology in 2004 was preceded by a strategic decision of SHMU to join the ALADIN consortium (www.umr-cnrm.fr/aladin/). By signing a Memorandum of Understanding in 1992, experts from SHMU and the academic sector became part of an international team involved in the ALADIN model research and development (R&D). ALADIN is designed as a version of the global model ARPEGE over a limited area (so called Limited Area Model - LAM). The development took place under the leadership of the French meteorological service Météo-France, which regularly provides data from the global model ARPEGE to consortium partners. These are used as the initial and lateral boundary conditions in the operational suites of the ALADIN models in many national meteorological services in Europe and several North African countries.

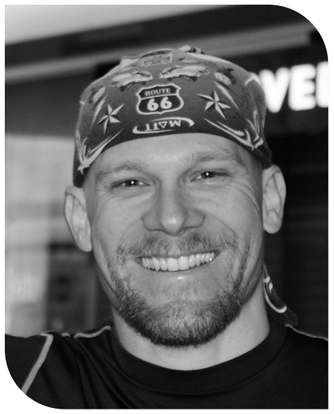
The source code of the ALADIN model has always been designed so that it can be run efficiently on different computer platforms. The model uses hybrid parallelization (a combination of MPI and OpenMP) and also includes an internal parameter that controls the length of the blocks with which the main computation loop is executed. This allows efficient execution of the model on HPC systems with different topology and scalar or vector computing cores. There is currently a single precision source code under development that is about 40% faster than the original double precision version. Adaptation of the model source code to the GPU architecture is planned in the near future. Emphasis is given to replace classical Fortran structures with an object-oriented model. This will simplify the use of the model with complex optimal estimation algorithms in the future.

The rights to operationally exploit the ALADIN model are subject to the obligation of SHMU to actively participate in the R&D of the model and on the maintenance of its source code providing 2 full time equivalents. Within Central Europe, the ALADIN member states decided to strengthen their cooperation beyond the existing ALADIN consortium memorandum, and in 1994 the RC LACE (Regional Cooperation for Limited Area modeling in Central Europe, www.rclace.eu) was formed with its own budget, management and mobility support among the members of the association. It is a unique example of Central European collaboration in the field of science with direct application of results into practice. Moreover, in 2021 a new consortium for NWP Cooperation in Europe named ACCORD has been formed. More details about the ACCORD can be found in the orange box below.

Slovakia had to wait for the first operational numerical weather forecast until 1st of July 2004, when it was launched on a high-performance computing system at SHMU.

SHMU is a member of ACCORD, the world's largest consortium focused on the research and development of numerical weather forecasts at a regional scales. ACCORD (www.umr-cnrm.fr/accord/) is a partnership of national meteorological services from twenty six European and North African countries including Slovakia. The key goal of ACCORD is to strengthen and share the research and development of a common code for numerical weather prediction and provide each member of the consortium with a state-of-the-art forecasting model that can be used for the operational weather forecasting at a high resolution.

Modern weather forecasts solve two basic tasks. The first task is the preparation of the initial conditions using measurements unevenly distributed in space and time by the optimal estimation methods, and the second task is to calculate the weather forecast based on known initial conditions. Problem

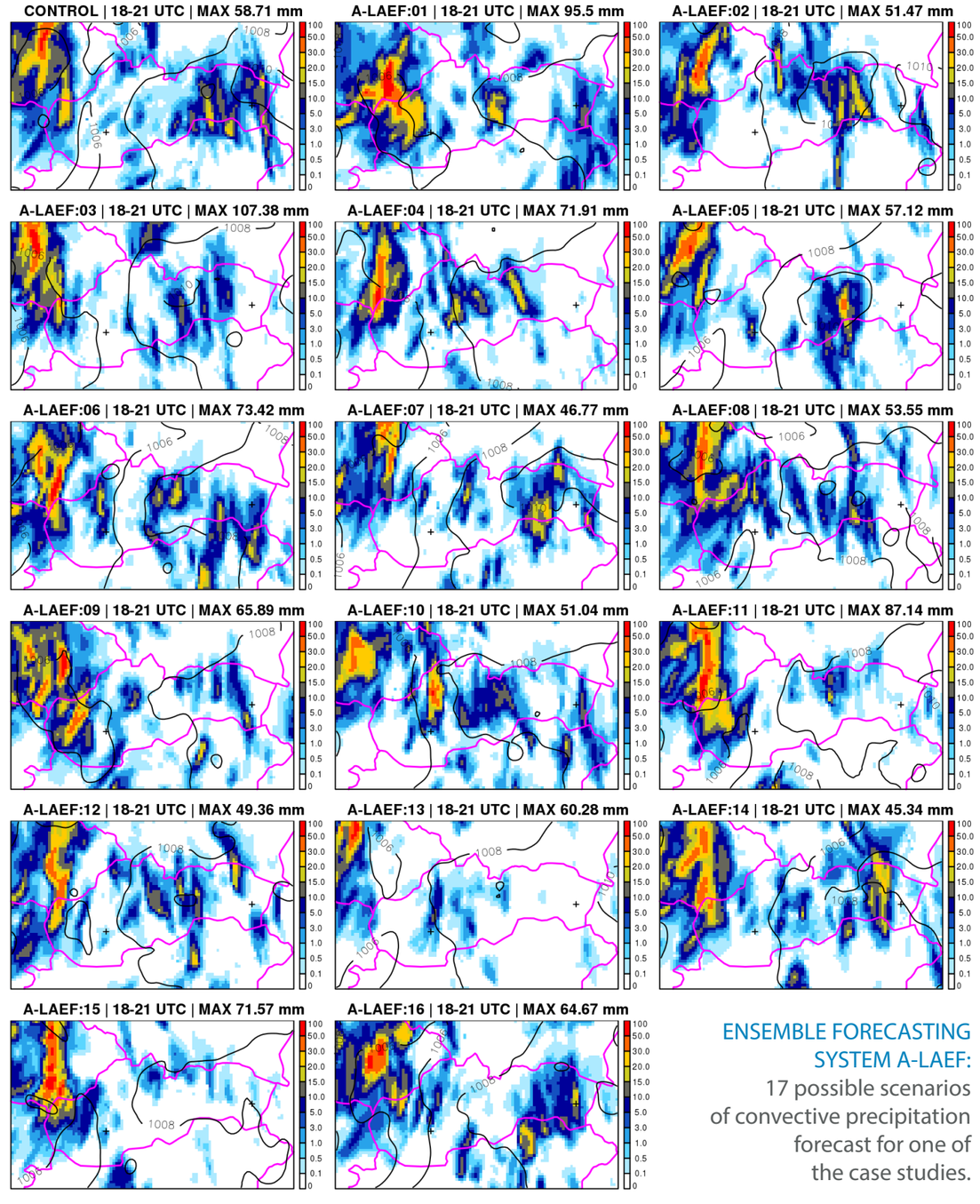


Martin Belluš is working at the NWP department at SHMU, and he is involved in the atmosphere predictability research. He developed and implemented into the operations an ensemble forecasting system A-LAEF that better captures extreme weather events in the next three days.

formulated in such a manner leads to a deterministic prediction. This type of forecast SHMU produces 4 times a day and makes products available to the general public for up to 3 days in advance with hourly steps. The most famous public products are the meteograms available on our web page.

Edward Lorenz discovered the chaotic nature of the behavior of dynamic systems in the second half of the 20th century. The weather forecast problem is a typical prototype of a chaotic system where prediction (in terms of time evolution of the atmosphere) calculated from very similar equally likely initial conditions can lead to completely different forecasts. This difference manifests itself on a time scale of several days, when it comes to large-scale phenomena such as atmospheric fronts and cyclones, and several hours, when it comes to organized convection, and even up to few tens of minutes, when summer storms are considered.

Therefore, the methods of NWP are gradually shifting from the deterministic approach to the probabilistic one, and so called ensemble prediction systems replace single deterministic forecasts. Ensembles are essentially a set of predictions calculated from equally likely, however a bit different initial conditions. The difference between the individual states of the atmosphere should correspond to the uncertainty of measurements, in other words to the measurement errors of individual meteorological parameters, such as temperature or humidity. In addition to the uncertainty of the initial state of the atmosphere, the uncertainty of the numerical model itself is simulated, because no model can describe reality without errors. This is done by using various physical schemes for individual members of the ensemble, but also by utilization of stochastic perturbations of contributions coming from the physical processes. Another method is to perturb the parameters themselves in different physical schemes, such as turbulence. The output of these systems is not only the expected value of the predicted variable, but also the probability of occurrence of the range of values. The advantage of the ensembles over the deterministic prediction is that it has the potential to capture even less likely scenarios involving extreme weather development. SHMU experts have played a key role in developing the A-LAEF (ALARO – Limited Area Ensemble Forecasting) ensemble prediction system



ENSEMBLE FORECASTING SYSTEM A-LAEF:
17 possible scenarios of convective precipitation forecast for one of the case studies.

operated by RC LACE on the ECMWF Supercomputer in Reading (CRAY XC30 system, with more than 3500 nodes with 36 computing cores on Intel Broadwell CPU technology). The A-LAEF ensemble prediction system consists of 16 perturbed members and 1 unperturbed control run, all with a horizontal resolution of 4.8 km and 60 vertical levels. The ensemble forecast is performed twice a day for the next 3 days. No RC LACE member has locally available comparable computing power to operate such an ensemble system over such a large computational domain.

After two upgrades of HPC HW in 2010 and 2014, there are currently 22 IBM nodes available at SHMU. These are 10 IBM p755 with 32 POWER7 type cores with 256 GB of memory per node and 12 newer IBM Flex p460 with POWER7+ cores. The available performance at SHMU has increased approximately 20 times since 2004. This allowed us to implement a surface observations data assimilation system and a blending by digital filter method which provides improved initial state of the ALADIN model by combining the local model prediction with the initial conditions of the global ARPEGE model. At the beginning of 2017, we implemented a version of the ALADIN model with a spatial resolution of 4.5 km x 4.5 km and 63 vertical levels. Within the next 10 years, global atmospheric models and relevant ensemble systems based on them will gradually reach these resolutions. Therefore, in the near future the numerical weather prediction strategy at SHMU shall follow two directions, according to the available computing resources. The resolution of the deterministic model shall reach approximately 1 km in horizontal and 100 or more levels in vertical. If the available computing power at SHMU permits, also the ensemble forecasting system at convection-permitting resolutions shall be implemented, albeit probably over a smaller computational domain. Forecasts at such resolutions will be updated more frequently, at least every 3 hours. The reason is that at these spatial scales the fast convective processes take place, winter valley inversions are formed, radiation fogs are initiated in interaction with terrain, air is cooled during winter above the snow cover and it flows into valleys and extremely low temperatures occur. For modelling and capturing these phenomena it is not sufficient only to increase the model resolution. We have to develop more accurate algorithms for radiation-cloud interactions, new approaches to the calculation of turbulence, and enhance algorithms describing the formation of clouds and precipitation. It is necessary to improve data that describes the characteris-

Mária Derková, PhD. is working at the NWP department at SHMU. Her research interest is in the area of data assimilation methods, she also supervises bachelor's and master theses at the Faculty of Mathematics, Physics and Informatics of the Comenius University in Bratislava.

Numerical weather forecasting and high performance computing are interconnected vessels that interact with each other.

tics of the Earth's surface and its interaction with the atmosphere. The RC LACE consortium and its ALADIN partners are working on the new ALADIN versions in order to improve the quality of forecasts in the near future, especially in terms of the above-described phenomena.

The installation of a new computing system is currently underway at SHMU. The cluster consists of two hundred and forty nodes, each populated with two Intel Xeon Gold 6230 twenty-core processors. Nodes will be connected by the OmniPath technology. According to the performance benchmarks that the suppliers were required to fulfill, we expect a thirtyfold to fortyfold performance increase compared to the current situation. This system will become available to the SHMU experts during the third quarter of 2021.

In addition, the air quality models will be operationally exploited on the new HPC system around 2022. We started development of interfaces between the ALADIN model and these atmospheric pollution models. The aim is to build an air quality warning system for the whole territory of Slovakia and not only at the locations where real-time monitoring is carried as it is nowadays.

In general, the higher the model resolution, the greater is the sensitivity to the initial conditions. Therefore, our main focus nowadays is on implementing methods that allow us to refine the initial conditions by using data that contains a high resolution meteorological signal, especially meteorological radars and satellites. We are currently involved in the development of radar data quality control and preprocessing for subsequent use in the process of preparing initial conditions. We test the use of new data sources, aircraft observations, ZTD (Zenith Total Delay) from satellite observations.

The biggest problem of strategic planning in the area of numerical weather forecasting in Slovakia is the absence of guarantee for regular renewal/upgrade of computing power at SHMU. We believe that this situation is based on a misunderstanding of the indirect economic value that high-quality weather forecasts bring. We have become accustomed to the fact that warnings and forecasts are available for free and their quality is gradually increasing. We subconsciously adjust our behavior according to this information, but we do not realize how much impact this information has on everyday life, on tourism, logistics, air traffic, radiation hazard protection, and generally on almost all our activities. The ALADIN model and its products have a transversal character in the Slovak economy. SHMU HPC infrastructure belongs to the critical infrastructure of the SR. However, there is no strategy to regularly renew computer technology directly from the state budget. At the same time, economic studies of the indirect economic value existing in other countries (USA, EU) show that every Euro invested in NWP will return more than ten times in the same year, while, for example, the return on highway investment is 5 times smaller.

Numerical weather forecasting and high performance computing are interconnected vessels that interact with each other. The complexity of numerical prediction models has always been limited by the available computing performance, in a way that the calculation of the one-day forecast must not exceed a few minutes. This rule still applies today, and we need high-performance technologies with performance tens to hundreds of Tflops in order to keep our activities at state-of-the-art level.

The future of NWP in Slovakia depends not only on SHMU, but especially on a sufficient number of well-prepared university graduates who will understand atmospheric physics, numerical mathematical methods and also be educated in programming methods on supercomputers. Such a goal falls beyond the SHMU scope of activities. We are very well aware that Slovakia needs to strengthen HPC centers that will be able to provide an education environment in the areas needed for NWP. This synergy slowly arises in Slovakia, and we believe it is going to be successful.

The biggest problem of strategic planning in the area of numerical weather forecasting in Slovakia is the absence of guarantee for regular renewal/ upgrade of computing power at SHMU.

03

HPC Popularization

hpc focus

1 National Competence Centre for HPC at ITAPA

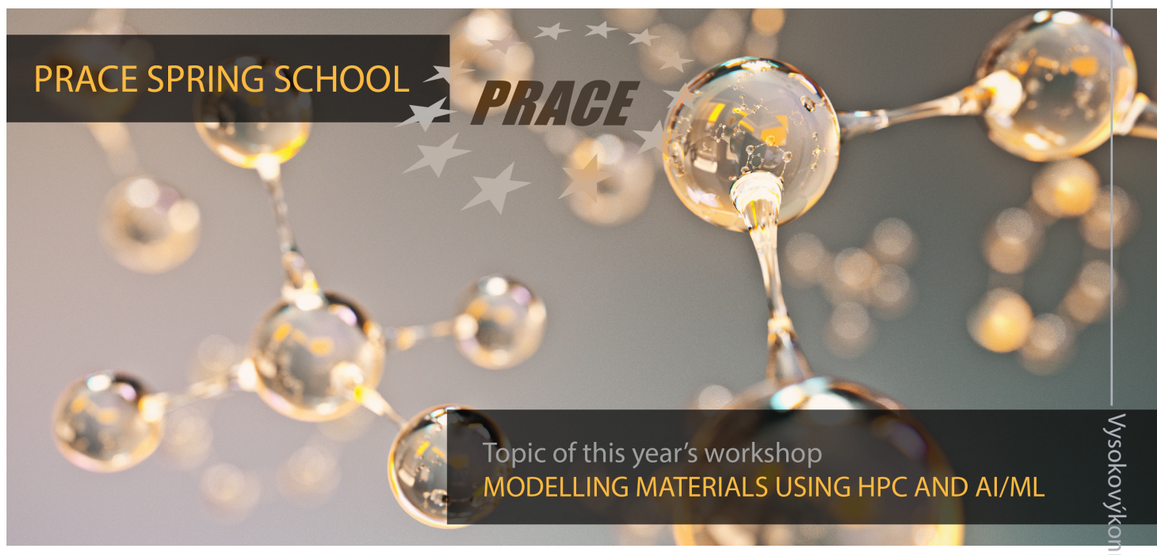
The 19th edition of the largest IT conference in Slovakia – **ITAPA** – took place on December 7 – 9, 2020. The **EuroCC** project and the **National Competence Centre for HPC** was presented by Lukáš Demovič, director of the **Centre of Operations** of the **Slovak Academy of Sciences** and Chairman of the Board of the National Supercumputing centre (NSCC).

In his presentation, L. Demovič introduced the scope and goals of the EuroCC project and underlined the importance of HPC in many areas, such as innovations, digitalization and transformation of industry. The National competence centre for HPC provides services for SMEs, industry, public and academic sector and enables them to utilize HPC, AI HPDA and ML tools in their business or research.

The newly founded National Supercomputing Centre (NSCC) was established in 2020 as a consortium of the Centre of Operations SAS, the **Ministry of Investments, Regional Development and Informatization** of the Slovak Republic and the **I4DI** organization. The NSCC is expected to cooperate closely with the NCC for HPC.

The importance and role of the basic and applied research in the transformation of industry was debated by L. Demovič during a discussion panel together with other participants, including the Deputy Prime Minister and Minister of Economy of the Slovak Republic, Richard Sulík.

2 PRACE Spring School



The mission of **PRACE** (Partnership for Advanced Computing in Europe) is to enable high-impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society. It was established on 23 April 2010 and is an international not-for-profit association (aisbl) with its seat in Brussels. It has 26 member countries whose representative organizations create a pan-European supercomputing infrastructure, providing access to computing and data management resources and services for large-scale scientific and engineer-

ing applications at the highest performance level. Slovakia is represented by Centre of Operations of the SAS – Computing Centre. Partnership for Advanced Computing in Europe regularly organizes PRACE Spring School.

This year the PRACE Spring school was organized by the Centre of Operations, Slovak Academy of Sciences and covered the topic of modelling materials using HPC and AI/ML tools and techniques. The workshop was held on June 15 – 18, 2021 as an online/hybrid event. Locally based participants attended the seasonal school in person.

We were very happy that several experts in the field participated in the Seasonal School: The VASP – Vienna Ab initio Simulation Package – team: Prof. Georg Kresse (University of Vienna, Austria), Dr. Martijn Marsman (University of Vienna, Austria), Dr. Martin Schlipf (University of Vienna, Austria), Dr. Ferenc Karsai (University of Vienna, Austria), Dr. Marie – Therese Hübsch (University of Vienna, Austria) with Tomáš Bučko (Comenius University in Bratislava, Slovakia) and Prof. Milica Todorovic (University of Turku, Finland).

This year PRACE Spring School was focused on material modelling from its theoretical concepts, implementation of parallel algorithms to effective use in HPC applications. One of the topics was dedicated to tools and techniques of machine learning. This method is nowadays more and more used to solve chemical problems and design new materials with specific properties.

3 Activities of National Competence Centre for HPC

Experts from National Competence Centre for High Performance Computing regularly organize free of charge IT courses on various interesting topics, which include parallel programming, work in HPC environment, neural networks, basics of Machine Learning (ML) and Big Data, programming and working with GPU/CUDA or OpenCL.

Currently National Competence Centre for HPC is preparing free of charge popularizing and educational lectures about High Performance Computing, launching in September. More useful information is on the webpage of National Competence Centre, where you can find current news from the world of HPC, new and future calls, information about courses, hackathons and other events.

Sign up for our newsletter, if you do not want to miss anything. Follow us on our social networks!

Experts from National Competence Centre for High Performance Computing regularly organize free of charge IT courses on various interesting topics.

PRACE

SEASONAL SCHOOL ON BIOINFORMATICS

One of the activities of the Computing Center of CoO (Centre of Operations) SAS within the **PRACE** project is to organize HPC-oriented workshops, so-called „seasonal schools". These workshops are organized typically four-times a year, each time by a different PRACE partner/country. The most challenging task for the host organization is to properly choose the topic so that it is both useful and attractive for the audience, and advertises HPC to new scientific communities. The Computing Center of CoO SAS already organized such workshop in January 2016 on the HPC implementation and efficient applications of Density Functional Theory in chemistry and solid state.

It is not only of PRACE but also our own ambition to broader the range of scientific fields that utilize HPC services. Due to growing popularity of bioinformatics and machine learning we decided to organize a seasonal school with a focus on these topics. During a few months of the workshop preparation we interviewed several research groups from institutes of SAS and Slovak universities. We tried to find out, which aspects and areas of the aforementioned broad topics are the most important for future participants. To our surprise, the overlap of interests (and software tools in use) was fairly small, which did not make the planning for us easy. Most of the interviewed groups were (so far) satisfied with serial applications that ran on a desktop or a (small) local computer cluster. Based on these findings we decided to focus the workshop on the most popular bioinformatics software package BLAST (Basic Local Alignment Tool) and generally applicable tools for big data processing (Apache Spark) and statistical analysis (language R) applicable in parallel HPC environment.

The workshop took place on 23rd to 25th of April 2018 on the premises of the Plant Science and Biodiversity Center of SAS, with the participation of 34 researchers from 13 institutions across Slovakia, Czech Republic and Austria. Prof. Erik Bongcam Rudloff from the Swedish University of Agricultural Sciences delivered an overview lecture "Introduction to Bioinformatics", that was followed by lectures and hands-on sessions by three experts from the Centre of Scientific Computing of Finland: Dr. Seija Sirkiä („Parallel programming in R"), Dr. Kimmo Mattila ("BLAST in HPC environment"), and Apurva Nandan ("Big data analysis using Apache Spark"). Participants could access the HPC computer cluster operated by one the SIVVP partners – Institute of Experimental Physics of SAS in Košice, during the workshop hand-on sessions. Unlike the Aurel supercomputer, this cluster is built on the x86-64 architecture that made the installation of required software stack much simpler.

Participants without prior experience with working in the HPC environment were offered a one-day long training course, that took place just a day before the start of the seasonal school. This training was lectured by Computing Center of CoO SAS staff, and participants could follow the lectures also remotely via teleconference.

Based on the feedback from participants of the seasonal school we can conclude that the event fulfilled most of their expectations. Our main goal was to attract wide spectrum of (current and future) HPC users, regardless if they used bioinformatics tools / methods already or if they plan to, and to inform the audience about the opportunities the Computing Center of CoO SAS has to offer.

Let us conclude by thanking Dr. Luboš Kľučár from the Institute of Molecular Biology SAS for numerous discussions and great help, not only with the selection of speakers.

Superheroes for SCIENCE

Visegrad Fund

High-performance computing and particularly supercomputing has become necessary for the advancement of all scientific fields, becoming the third pillar of science after theory and experiment. Popularization of the importance of supercomputers and their use for the improvement of people's everyday lives is very important and necessary.

The goal of Superheroes4Scienece is to explain the fundamental role supercomputers play in innovations and scientific advancements, the advantages of their use, and to highlight how they influence everyday life. The project explains what HPC means, how it works and how it is used with examples from everyday life. State of the art computational technology and research should inspire the target audience or at least improve the transparency of HPC deployment.

Each partner of the project represents one of the countries of the Vysegrad group. They are the **Computing Center of the Center of Operations of the Slovak Academy of Sciences (Slovakia), Governmental Information-Technology Development Agency (Hungary), IT4Innovations National Supercomputing Center at VSB – Technical University of Ostrava (Czech Republic) and Poznan Supercomputing and Networking Center – Institute of Bioorganic Chemistry of the Polish Academy of Sciences (Poland)**. Each project partner currently operates a national supercomputing infrastructure, and invests great effort into popularization activities in order to explain what supercomputing really is, why it is essential in today's society, and why it is a justifiable investment.

The understanding of both scientific topics and supercomputing is not easy for non-experts. To make all communications understandable, we tailored all dissemination materials for various levels of age, education, and expertise. The aim of the project is not only to educate the general public, but also to inspire the younger generation in V4 countries to take up careers in science, engineering, technology and mathematics. More graduates of these disciplines are needed not only as the administrators of the HPC infrastructures, but also as the perspective users of the real Superheroes 4 Science: the supercomputers.

Do you want to know more?
superheroes4science.eu
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instagram.com/superheroes4science

hpc focus

2021

DIRECTOR of CoO SAS
Lukáš Demovič

RESPONSIBLE REDACTOR
Lucia Demovičová

GRAPHIC DESIGN & DTP
Gabriela Obadalová

PHOTOS
Pavol Novák
Shutterstock

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Computing Center
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845 35 Bratislava
Slovak Republic
Tel.: +421 (0)2/3229 3111
Fax: +421 (0)2/3229 3103
E-mail: vssav@savba.sk
www.vs.sav.sk

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Computing Center

Dúbravská cesta 9
845 35 Bratislava
Slovak Republic

www.vs.sav.sk

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