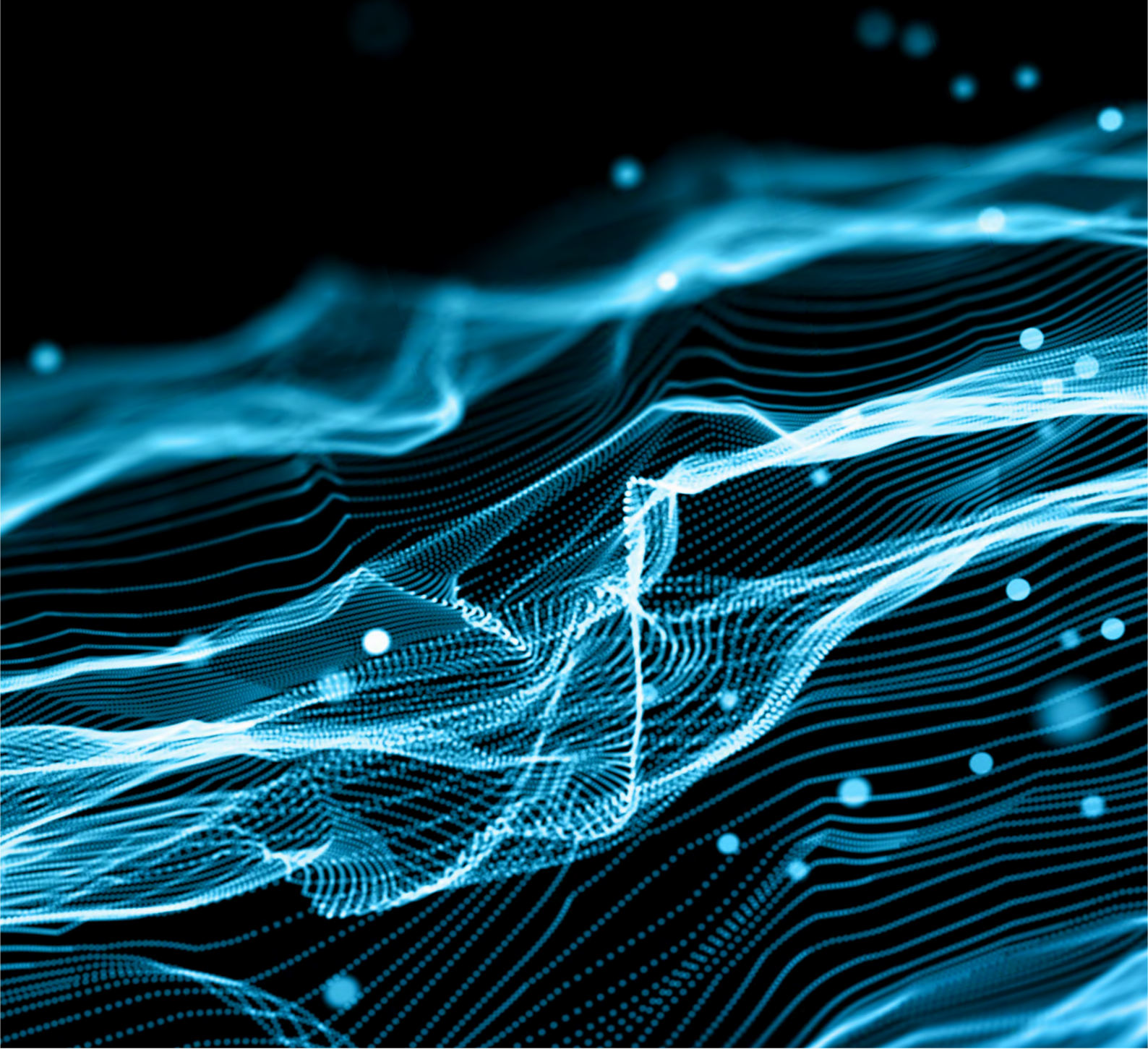
HPC @hu

HPC Competence Centre



SUPERCOMPUTERS IN HUNGARY

2001

Type: Sun E10k (Budapest)
Performance: 60 GBops
Number of CPU cores: 96
48 GB memory
TOP500 (Ranking: No. 428)

2011

Type: SGI UltraViolet 1000 (PŽcs)
Performance: 10.5 TBops
Number of CPU cores: 1152
6 TB system memory
500 TB disk capacity

Type: SGI Altix ICE 8400 (Debrecen)
Performance: 18 TBops
Number of CPU cores: 1536
6 TB memory
500 TB disk capacity

Type: HP CP4000BL (Szeged)
Performance: 20 TBops
Number of CPU cores: 2400
6.6 TB memory
250 TB disk capacity

Type: HP CP4000SL (Budapest)
Performance: 5 TBops
Number of CPU cores: 768
2 TB memory
50 TB disk capacity

2015

Type: HP SL250s (Budapest)
Performance: 27 TBops
Number of CPU cores: 280
882 GB memory
500 TB disk capacity

Type: HP SL250s (Debrecen-LEO)
Performance: 254 TBops
Number of CPU cores: 1344
10 TB memory
585 TB disk capacity (together with that of Apollo)
TOP500 (Ranking: No. 308)

Type: HP Apollo 8000 (Debrecen-Apollo)
Performance: ~106 TBops
Number of CPU cores: 1080
5.6 TB memory
585 TB disk capacity (together with that of LEO)

Type: SGI UV 2000 (Miskolc)
Performance: 8 TBops
Number of CPU cores: 352
1.4 TB memory
240 TB disk capacity

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Not only should one look like fast, one should actually be fast

It is normal human behaviour to strive for the gold medal everywhere, and digitalisation and infocommunications are no exceptions to this either. In this accelerated world of ours, exchanging data, understanding data, and analysing data are of particular importance since running a complex mathematical operation or understanding a relationship may even save lives but may also have a significant effect on the economy. The Hungarian Government aims to implement innovative development projects in this sector to further boost the national economy and to further expand the number of technological services available to the industry and the general population.

I am proud that under the leadership of the Ministry of Innovation and Technology, the Governmental Agency for IT Development – an organisation with more than 20 years of experience – has initiated the supercomputer development projects forming the basis for establishing future solutions. In addition to improving the HP infrastructure, KIFU will pay special attention to establishing supercomputer competences in order to provide value-added services for our users in the future.

It is a key objective to see Hungary among the pioneers of technological development, for which we have the necessary basis as much now as we had throughout history. Our outstanding professionals, researchers, and innovators continue a work, which carries forward the intellectual legacy of the internationally recognised Hungarian scientific community. Another of our objectives is to reappear on the map of countries providing the largest supercomputer capacities, and to thereby support the Hungarian research base and join international cooperation projects that enable us to participate in successful worldwide collaborations.

From science to innovation

Dr. Károly Balázs Solymár
Ministry of Innovation and Technology
Deputy Secretary of State for Digitalisation

Supercomputing looks back to a history of almost 50 years but has never been in the forefront of interest so much as exactly nowadays. Technology advances at a speed of wind, and the application of HPC has already emerged in every area where considerable research/development/innovation is involved. The developed regions of the world are competing to build ever stronger supercomputers and to conquer novel areas of use. In the near future, highly significant and exciting HPC investments will be implemented both around the world and in Europe, and an efficient utilisation of the resources is also assisted by new forms of international collaboration. Whoever is missing out will inevitably fall behind. As regards competitiveness, innovation, and development. This is something Hungary cannot afford either. That is why it is so important that supercomputing in Hungary – which boasts of a beautiful history and a great number of success stories – is on the brink of a decisive development again, which includes both a renewal of the infrastructure and an improvement of the associated services to a new and higher level.

Within KIFU, the Hungarian HPC Competence Centre started to operate in 2020 with the help of EU funds; the most important task of this centre is to promote the widespread and efficient use of supercomputing in Hungary as much as possible. The Competence Centre discharges its duties with the involvement of, and in close cooperation with, the affected institutions, and this is also assisted by an international cooperation as part of the network of European of HPC Competence Centres. This introductory publication provides information on where it all started, and how and where we would like to end up in the period to come.

Dr. Tamás Máray
Head of the HPC Competence Centre
Governmental Agency for IT Development (KIFU)

Supercomputers in Hungary – *we are keeping up with the world*

Following the example of the developed countries, the idea that Hungarian scientific life would also need supercomputers emerged in Hungary for the first time in the region already during the late 1990s. The National Institute of Meteorology already used a special, dedicated device, and upon surveying the needs, all major Hungarian players – scientific universities and the institutions of the Hungarian Academy of Sciences – concluded that supercomputers are also indispensable for scientific research.

A new era

In 1986, the Information Infrastructure Development (IIF) Program was launched with the objective of establishing and operating the central infrastructure of research, academic education, and public collections. In 1992, the operation and development of this central infrastructure was transferred under the powers of the National Information and Infrastructure Development (NIIF) Program. In the meantime, the number of users and areas of use grew exponentially, and the need for a supercomputer emerged.

After an invitation to tender in 2000, a SUN Microsystems supercomputer with a performance of 60 gigaflops was delivered to Budapest in 2001, and became available for Hungarian researchers and academic education already during the same year. In addition to the infrastructure, a group of professionals also responsible for support, advisory, and even educational tasks was organically formed within the NIIF Institute, and became the predecessor of the current Competence Centre (CC).

Upon this investment, Hungary became included in the list of the top 500 largest supercomputers in the world. The development project gained international interest, and delegations also came from Austria and Czechia to learn about this technology via consultations with the Hungarian experts having first-hand experience. Universities and research institutes immediately recognised and made use of the capabilities of the supercomputer, and the increasing demand resulted in further capacity expansions.

Develop, expand, and keep pace

The Hungarian supercomputer infrastructure had matured into one with an increasingly imposing performance in several phases, and had been almost completely renewed by the early 2010's.

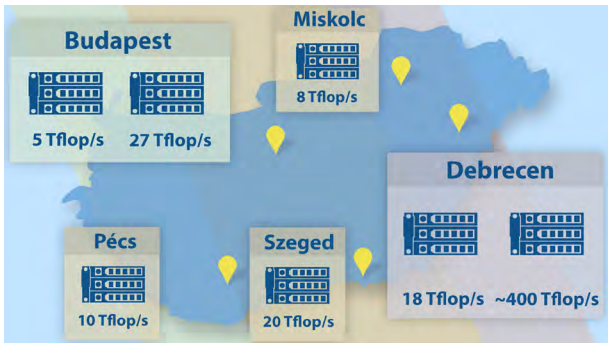
This infrastructure was highly reliable and exceptionally fail-safe; what is more, the Sun Center of Excellence, which participated in the operation thereof in the form of a partnership, awarded a plaquette for the work of the predecessor of KIFU.

Projects with the participation of several hundred researchers – including non-Hungarian researchers – were completed, and the feedback from professional events organised for the users and from 1- to 3-day workshops involving international lecturers, clearly indicated that the available capacities are not sufficient any more.

Meanwhile, needs continued to increase at a dazzling speed making it indispensable to achieve a profound renewal both in terms of technology and of performance, that is, a completely new infrastructure was required.

A distributed infrastructure is being built

Then, the scientific universities of Debrecen, Pécs, and Szeged concluded an agreement with the NIIF Institute to host supercomputers. Accordingly, the universities provided machine room capacities for the supercomputers, and also bore a portion of the operational costs. The investment partially financed from EU funds, as well as the operation, fell under the powers of the NIIF Institute.



By 2011, a completely new infrastructure consisting of 4 supercomputers was built. Computers with a performance of 10 to 16 teraflops were installed in new buildings in Debrecen and Pécs, and in the existing machine room in Szeged; the fourth machine with a performance of 5 teraflops replaced the previous SUN supercomputer in Budapest. In the form of a distributed HPC infrastructure connected to the high-speed optical backbone grid of the research institutes, these supercomputers served and still serve science: researchers, academic education, and public collections.

2011 was a turning point in every aspect: on behalf of Hungary, the NIIF Institute – the predecessor of KIFU – joined an international supercomputer user and developer collaboration established with support from the European Union.

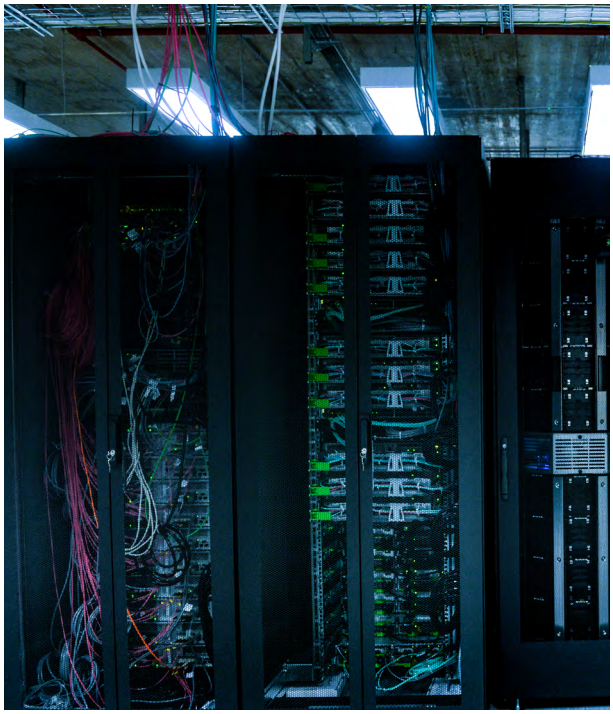
Complete transformation

During the integration into the international frontline, supercomputer capacities in Hungary were kept updated, developed, and increased. In 2015, two new supercomputers started to operate in a new building in Debrecen, and another two in Miskolc and Budapest. The aggregated performance of the entire Hungarian supercomputer infrastructure was 0.5 petaflops then. Thus, Hungary had 8 supercomputers in 2016, 4 older ones and 4 new ones; however, feedback indicating a demand for additional capacities was being received again at an increasing frequency.

A pre-development survey among the users unequivocally demonstrated that a complete renewal is inevitable. The distributed infrastructure – several locations and several parallel operational tasks – proved to be too subdivided, and thus a decision to concentrate the supercomputer capacities was made.

Hitting a new level: capacity expansion and concentration

Thanks to the ongoing development projects, a supercomputer with a computing capacity of 5



petaflops will be available for researchers and industrial players from 2022. Metaphorically speaking, this new computer is a jump into the future: its independent performance represents a 10-fold increase in comparison with the previous distributed infrastructure.

Upon a detailed restructuring of the Supercomputer Centre at the campus of the University of Debrecen, the unstoppably increasing needs will be primarily satisfied by this newest Hungarian supercomputer. Thanks to this development project in a value of HUF 6 billion from EU funds, the opportunities for supercomputer use by the Hungarian scientific community and economic sector will increase by several orders of magnitude. Another fact reflecting the extent to which capacities are being increased is that Hungary may again land on the top 500 list of supercomputers – for a time.

The Supercomputer Centre of Debrecen

Ybl Prize- and Pro Architectura Prize-winning architect, Marcel Ferencz specifically designed a two-storey building with a footprint of 400 m2 at the campus of the University of Debrecen to host supercomputers. The ground-floor has a server room with a footprint of 150 m2, and the first floor has an area of 70 m2 for the research laboratory and a working station in addition to the electric and engineering areas. The cooling units of the supercomputer are located in separate engineering areas.

The building uses modest, cost-effective, and simple materials. The main facade has a relief showing the function of the building, which is thus a worthy, statue-like member of the series of buildings of the university campus.

HPC @hu
Competence Centre

The HPC Competence Centre

The use of supercomputers is extremely complex, and therefore, it cannot be expected from people other than specialists working in the IT field to understand every minute detail thereof. This inspired the creation of the HPC Competence Centre; this organisational unit was established in 2020 with the main objective of promoting and supporting a more efficient and successful use of the supercomputer infrastructure in as wide a scope as possible. In order to achieve this, the Competence Centre pursues several activities: providing high-level user support, consulting, advisory services, and trainings required for the use of supercomputers, as well as disseminating an HPC culture. To this end, the centre cooperates with those institutes of academic education where professionals from the fields of sciences with an inevitable use of HPC are trained. Thus, the objective is to establish and operate an HPC ecosystem of European quality in order to support scientific research, academic education, and market/industrial innovation in Hungary.

A supercomputer infrastructure is of exceptional value but the maintenance and operational

costs thereof are high at the same time; therefore, a single institution could hardly finance it. Consequently, it is an established global practice to create national supercomputer centres that serve a wide range of user institutions. During the second quarter of 2020, the HPC-CC Coordination Office of the Governmental Agency for IT Development (KIFU) conducted a survey among existing HPC users from the academic sector.

The development and operation of the national HPC resources is a key duty of KIFU. By today, supercomputers – that is, the HPC infrastructure – have become one of the most universal research tools. The use of HPC is present in all scientific fields; in addition, this tool is one of the engines of industrial innovation. Owing to this urgent recognition, the years to come will witness the IT investment of the decade in KIFU in a value of HUF 6 billion, and with support from the Ministry of Innovation and Technology. Upon this renewal of the infrastructure, research & development in Hungary will gain new impetus, and several international collaboration opportunities will be enabled. Our objective is to purchase a modern supercomputer with a performance of at least 5 Pflops, and to provide top-quality services and support to the users.

Upon an initiative of Mr. László Palkovics, Minister of Innovation and Technology, KIFU established an organisational unit dedicated to provide support for supercomputer users – i.e., the Competence Centre – in early 2020.

The real added value comes from the high-level and complex user support provided during the use of the supercomputers. Just think about it: a researcher does not necessarily have the IT skills required to run his/her project on a supercomputer. However, we do not want to dissuade anyone at all from using supercomputers because of a lack of high-level IT or programming skills. Therefore, 5 levels of user support were defined to match the different levels of IT and programming skills the users may have. This user support also includes case management, such as the management of general (non-technical) requests, or answering questions emerging in relation to the requests for project allocation. Technical issues, such as access problems and running difficulties, are also resolved here. The services also include the installation of new software products, the scripts required for the runs, the wrong resource uses identified during the runs, and the provision of information to the users. In addition to the above, consulting services are also provided to our new users, and we also try to ensure support in application and algorithm development issues; however, we may still provide assistance through our international relations even if the need of a user cannot be fully satisfied by the Hungarian infrastructure.

Our HPC portal, which actually represents a single-window administration system, is under ongoing development. This is where the requests for project allocation are submitted and the assessments thereof are received, and the portal also functions as a quasi-dashboard to inform users on project statuses, and to transmit maintenance and system messages.

One important new element in our activities is the issue of training and education. Currently, we are working on our training portfolio for 2021. As yet, these are only planned in a virtual format but as soon as it becomes possible, in-person trainings and workshops are also envisaged. Topics are selected on the basis of the feedback from our users.

Although the CC Team is strengthened by HPC

experts, with a view to meeting user needs on a higher level, a model integrating experienced HPC users from various fields of science was created in order to enable them to help with the project allocation procedure and the running processes with their expertise. Their skills are of vital importance because each discipline has its own special knowledge and methods, and the translation thereof into the language of supercomputers is not a trivial task at all.

In everyday practice, the experts of the HPC Competence Centre are responsible for the management of the user demands received, that is, they are the managers of the resources of the national HPC infrastructure. Therefore, the HPC Competence Centre ensures a high level of user support, and liaisons with both Hungarian users and international professional partners. At the same time, the KIFU HPC Competence Centre represents the Hungarian HPC infrastructure and community at international professional forums.

The TOP 500 is our target

Development of the supercomputer infrastructure

The preparations for the installation of the newest Hungarian supercomputer clearly illustrate the complexity of developing an HPC infrastructure, the need for planning with a sense of perspective, and the challenges the experts of KIFU will face. For the installation of a supercomputer with an exceptionally high performance, which is used for special research and innovation purposes, almost everything had to be refurbished in the Supercomputer Centre of Debrecen, except for the building frame.

By 2022, a supercomputer with a computing capacity of 5 PF will be available in Hungary, which represents a 10-fold increase in comparison with the current infrastructure. The CPU, GPU, MI, and Large-memory partitions will include more than 40 thousand processor cores and 400 GPUs, and this will be completed with a high-performance temporary storage and a high-capacity long-term storage. These together with the most advanced translating and licensed scientific software products result in a leading-edge research infrastructure.

Many computing units are needed to achieve the high performance of supercomputers but the most advanced types are also characterised by a high performance density, and therefore, do not need extremely large spaces; this is how it is possible to host a supercomputer with a >10-fold higher performance within the same space. However, the associated accessory pieces of equipment require space and unique engineering solutions. Another important aspect is that supercomputers often work at maximum performance as they are dedicated machines with rapid obsolescence that lack safety margins,

and thus always have to offer peak performance. Accordingly, the energy consumption thereof is huge; cooling itself is extremely expensive, and the new supercomputer thus requires a new power-current supply system.

In order to reduce the cooling costs, a special, so-called "warm-water cooled" HPC is being built. The parts and other elements are cooled without compressors, by using a liquid at a temperature of 32°C, and applying adiabatic (fan-based,water sprayingenhanced) cooling technology; that is sufficient to ensure a high-speed blow-through of outside air to achieve the required temperature. This warm-water cooling technology is one of the first such solutions in Hungary and is highly environment-friendly; another considerable advantage thereof is that the heat generated within the system can easily be removed and recycled. Both the city and the university are open to this as they are in search of the best solution for the utilisation of the waste heat (e.g., hot water production and heating of the campus buildings resulting in a saving of more than HUF 10 million).

With the new supercomputer – named Komondor as a result of a voting –, KIFU will become the backbone that served academic education, public education, research & development, libraries and public collections, and several other public institutions in Hungary, and will communicate with the outside world at a bandwidth of 100 GB/sec through the HBONE+.

Since an uninterrupted operation is extremely important in case of a supercomputer, power outages should be immediately remedied by switching to battery supply for not only the machine itself but also for the associated infrastructure and the cooling system. If in turn, the room-sized batteries run down, a diesel engine-operated electric generator is switched on. In case the power supply cannot be restored even during the time thus gained for any hardly conceivable reason, the supercomputer enters the emergency operation phase, followed by a gradual shutdown. In the same manner, we should be prepared for all types of risks: when experts from the manufacturer or KIFU do repair works on the supercomputer, they will be grounded to individual grounding points to eliminate the risk of damage caused by an electrostatic discharge. In case of fire, a supercomputer cannot be extinguished with water or foam, and thus oxygen – which is indispensable for burning – is simply displaced and expelled from the machine room by a system using a special gas.

With this development, which is expected to be completed by the summer of 2021, we will reach the physical limits of the building: it can host no more high-performance devices beyond having a maximum power supply. The large spatial needs of the associated infrastructure, including the 7-tonne cooling equipment, and other features of the system constitute a bottleneck, and delimit the potential for future developments in the machine room.

TOP 500

This project provides a classification and a detailed analysis of the 500 non-distributed supercomputer systems with the highest performance in the world. The dazzling speed

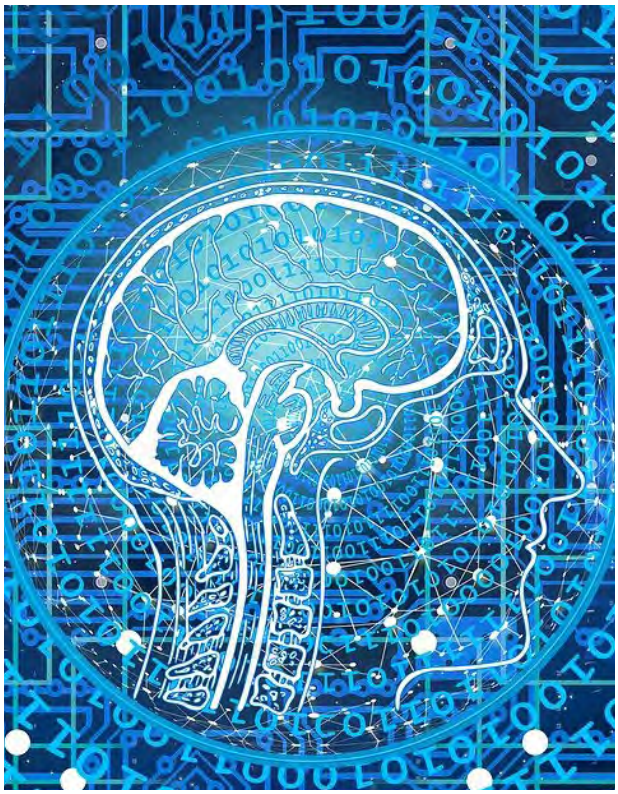
of the development of supercomputers is also reflected by the fact that this ranking has been updated twice a year since 1993.

Adiabatic cooling

The basic principle of operation is very simple: evaporating water removes heat from its environment. A warmer and drier air can absorb more water vapour, that is, performance increases in proportion to the temperature.

Komondor

Komondor is one of the most well-known breeds of Hungarian sheepdogs. It is an incorruptible, assertive, and brave protector. Safeguarding the herd from predators and thieves, and not shepherding was the task of this breed. During guarding at night, Komondors were distinguished from attackers by their white colour. They are fast learners and have an exceptional applied intelligence, and that is why the newest Hungarian supercomputer was named Komondor in 2020.



International cooperation for competitiveness – collaboration in the area of developing and using supercomputers

Our role in the international HPC circulation

All around the world, the academic/scientific research community was the first to promote the use of supercomputers, and the related communication and exchange of experience was running along its known formal and informal ways: via conferences, workshops, publications, and, of course, personal exchanges. However, the knowledge and the unknowns related to supercomputing pried these frameworks of liaison and communication. Scientists, researchers, and industrial players emerging as interested parties and potential users showed an ever increasing and urgent need for a comprehensive and intensive support, since high-level IT and programming skills are required for achieving the desired results. That is why an HPC Competence Centre was also established in Hungary, under the management of KIFU.

The HPC Competence Centre liaisons with international professional partners, and also represents the Hungarian HPC infrastructure and community at international professional forums. The HPC Competence Centre is an active participant of several international initiatives and projects.

PRACE (Partnership for Advanced Computing in Europe) is a joint European supercomputer infrastructure and cooperation program established in 2010 with support from the European Union. The main objective of PRACE is to ensure a wor-

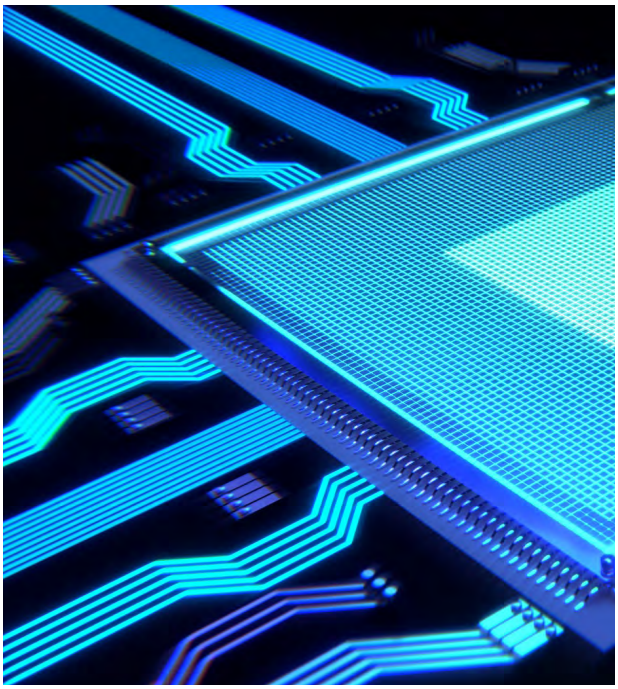
ld-class infrastructure for European research & development and innovation efforts free of charge, which guarantees Europe's competitiveness in comparison with other developed regions of the world. One objective of PRACE is to improve its services, efficiency, and the quality of user support, and to enhance cooperation between European supercomputer centres. KIFU has been the representative of Hungary in PRACE since 2011. The participation of KIFU in the PRACE project is of vital importance because this provides a framework for gaining access to European leading-edge technologies, and for taking part in professional collaborations and EU-supported projects that are fundamentally required in order to maintain and improve the quality of HPC services in Hungary.

Europe versus the world – A continental cooperation

Although the PRACE cooperation and the various national HPC programs and projects conducted in EU countries resulted in a significant development in supercomputing in Europe during the past decade, our continent still could not keep up with the more rapidly advancing USA and with the Far East region coming up at extreme speed (China and Japan). These are well reflected by both the relevant statistics and the fact that the above-mentioned countries declared the strategic importance of supercomputing years ago, and launched programs to reach performances in the exaflops range by allocating significant funds for this purpose. As a result, three supercomputers with performances exceeding 1 exaflops are to be commissioned in the USA during 2021, and China announced similar investments. Upon recognising that this fallback represents a handicap for Europe, the EU established the EuroHPC Joint Undertaking in 2018. Currently, 33 European countries share their resources with the EU and with the industrial players to ensure a world-leading position for the EU in terms of supercomputing. The mission of the EuroHPC JU is to develop, install, expand, and maintain world-class, integrated supercomputers and data infrastructures, and to develop and support a highly competitive and innovative HPC ecosystem in Europe.

One objective of the EuroHPC Joint Undertaking is to provide the EU with a petascale infrastructure by 2021, to prepare for building exascale supercomputers, and to elaborate on the technologies and applications required for the use thereof by 2022/2023.

A coherent and consistent objective of the EuroCC and CASTIEL projects established under the aegis of the EuroHPC initiative is to ensure a high level of expertise throughout Europe in the area of HPC and the related fields of science, such as high-performance data analysis (HPDA) and artificial intelligence. Such knowledge and expertise are of vital importance in order to maintain and strengthen the technological autonomy and global competitiveness of the European Union.



The EuroCC Project

This project is run under the aegis of the EU Horizon 2020 (H2020) with the participation of the national HPC Competence Centres of 33 countries including the HPC Competence Centre of Hungary. These centres coordinate all supercomputer-related activities on the national level, and liaison with the scientific community and industrial players,

existing and future HPC experts, and the general public. The competence centres also collaborating with each other under the framework of the EuroCC Project facilitate the access to European HPC resources by offering customised solutions for a wide range of users, including researchers and scientists, public administration, and various industrial/market players. The EuroCC Program is funded by the H2020 Program and the partner countries in a ratio of 50% to 50%.

The CASTIEL

The CASTIEL Project promotes interaction and an exchange of experience within the EuroCC network. The project experts are developing a competence map for the whole of Europe, which will show the resources available in each centre and identify the points of improvement. This will encourage potential collaborations, the exchange of well-established practices, and the sharing of knowledge and expertise. The CASTIEL Project will coordinate activities such as international workshops, various partnerships, thematic work groups, and addressing questions of mutual interest. The HPC Competence Centre is indirectly involved in this project.

LEONARDO

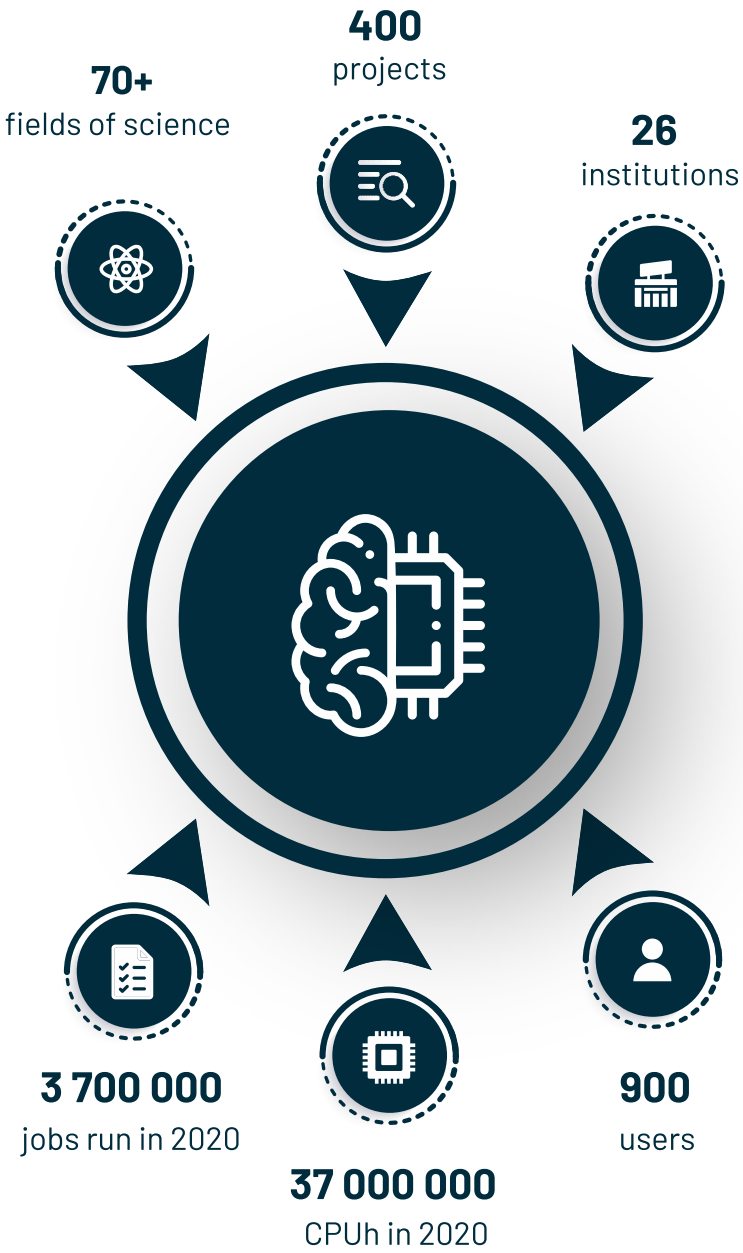
Under the framework of the EuroHPC Program, one of the most powerful supercomputers with a performance of 250 petaflops and the name Leonardo will be completed by 2021 in Bologna with joint funding from the EU and Italy. Leonardo will be one of the 3 supercomputers with pre-exa performance in Europe (the other two being LUMI in Finland and Mare Nostrum 5 in Spain).

The Leonardo Project is funded by the EuroHPC JU on behalf of the EU and by the Ministry of Education and Research on behalf of Italy in a ratio of 50% to 50%. The project is being implemented by the Italian national supercomputer centre referred to as CINECA. Furthermore, Austria, Slovenia, Slovakia, Greece, and Hungary are also official consortium members providing expertise for the project. The knowledge of the experts from KIFU is a contribution to the success of the project. In an exchange for the resources offered, the supercomputer capacities created will also be available for Hungarian users.

During the past two decades, Hungary also witnessed the use of supercomputers becoming not only exceptionally useful but inevitable in an increasing number of areas. The Competence Centre continues to work on utilising the advantages of its rich international relations to the benefit of our users, and on expanding the areas of use.

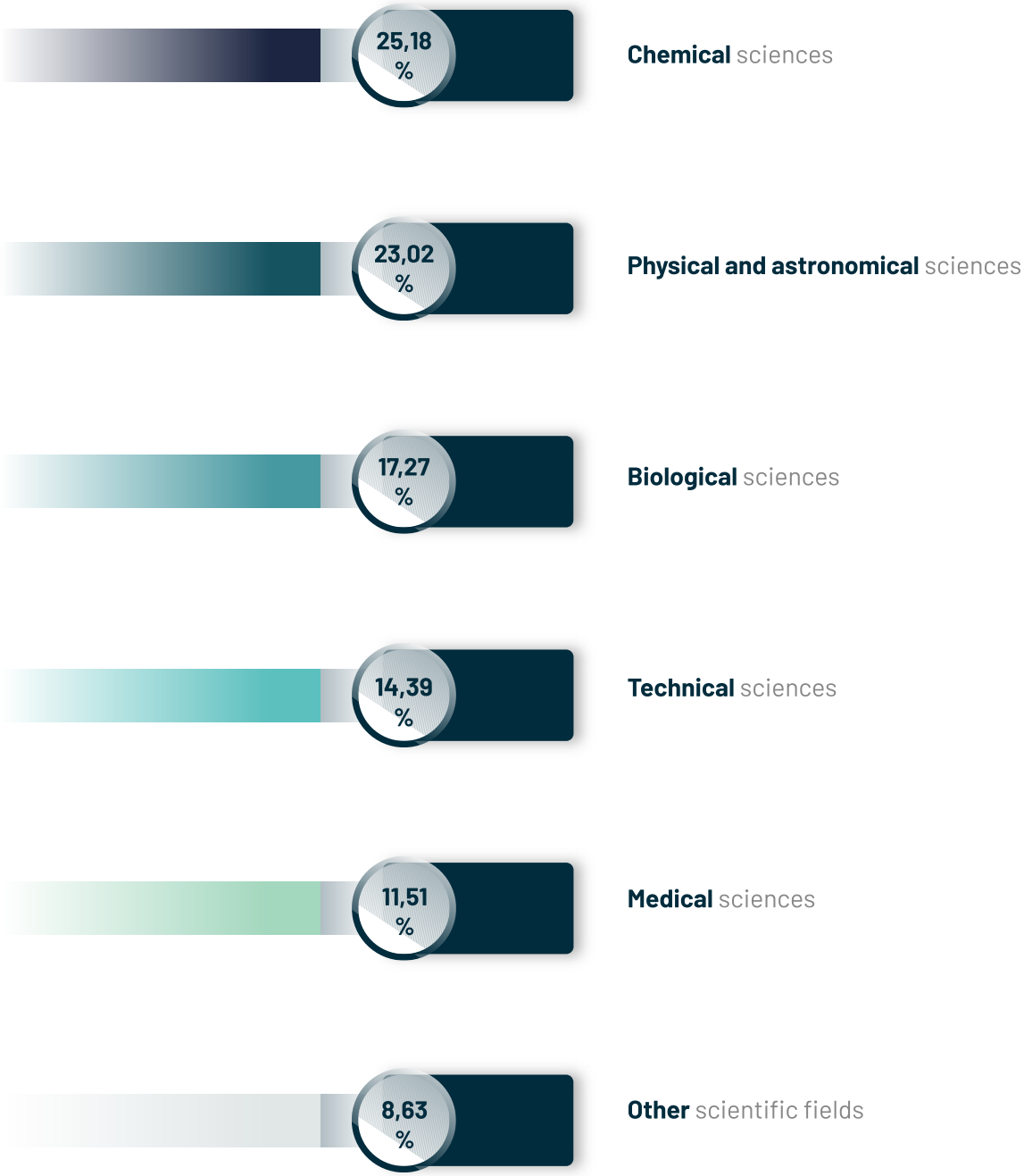
HPC uses in numbers

There exists a wide range of uses of supercomputer capacities. We almost have a thousand HPC users from a total of 26 research institutes now. This high-performance infrastructure serves experts from several fields of science and more than 400 projects. The several million jobs that were run helped researchers in many of their scientific achievements.



Fields of research

Among the fields of research using supercomputing resources, STEM (Science, Technology, Engineering and Mathematics), that is, natural and real sciences including highly significant medical scientific uses, are typically at the highest ranks in Hungary too. Other categories include representatives from agricultural sciences, geological sciences, and even linguistics and literary sciences.



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For further information, please visit the website **hpc.kifu.hu**.
Please, send your questions to **hpc@kifu.hu**.

EURO
ACCESS

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