Academic Computer Centre

CYFRONET AGH

2025

ACC CYFRONET AGH is a leading unit empowered by the Committee for Scientific Research to develop and manage the High-Performance Computers (HPCs) and Cracow Metropolitan Area Network (MAN). CYFRONET is the coordinator of the PLGrid Program and is recognized by the National Centre for Research and Development as a Centre of Excellence in the area of grid and cloud services.

Dear Readers!

Another year has passed of intense work to provide our Users with the latest technologies to support the development of Polish science, innovative economy, and information society.

With the launch of Helios, which took over from Athena as the fastest supercomputer in Poland, we have significantly expanded the capabilities of performing advanced computational tasks, including the development of artificial intelligence. Helios has 35 PetaFlops of theoretical computing power, mainly from graphics processors, which allowed, among other things, the effective support of creating Polish language models Bielik and PLLuM. On the November Top500 list of the fastest supercomputers in the world, Helios was classified twice, including as a GPU partition in a high 69th place. Athena and Ares were also noted on the same list, meaning that half of the eight positions occupied by Polish machines were supercomputers operating in Cyfronet.

However, it is worth noting that we care not only about the development of computational capabilities but also about their most efficient use, considering environmental issues. This is confirmed primarily by the classification of the GPU partition of Helios on the prestigious Green500 list of the most energy-efficient supercomputers in the world, where it took 7th place. Considering that on the previous edition of this list, Helios was ranked 3rd, and Athena was noted at 10th place in 2022, we can boldly say that the supercomputers we build are among the most efficient machines in the world, and our competencies in optimising systems and software are at the world level.

At the same time, we enter the next year of activity by actively participating in many other initiatives. Cyfronet organises competitions for one-year access to computations on the LUMI supercomputer, Europe's third most powerful supercomputer in late 2024. Additionally, thanks to representing Poland in the international LUMI-Q consortium, the Helios supercomputer will be directly connected to the quantum supercomputer being built in the Czech Republic.

All the resources mentioned are available within the PLGrid infrastructure initiated and coordinated by Cyfronet. The strategy of unifying access to various resources within the PLGrid infrastructure, adopted years ago, has brought many benefits to users. After logging into the PLGrid Portal, you can easily choose from many machines, virtual environments, and software packages. The Helpdesk team, or the Operational Center, provides invaluable support, and Cyfronet also organises training sessions for users on the effective use of the tools provided. In this regard, it is worth mentioning the coordination by Cyfronet of the National Competence Center in HPC, created jointly with other HPC centres in Poland, which serves as a contact point for computational services for scientists, startups, small and medium-sized enterprises, large companies, and public administration.

In 2024, we started another project in the series modernising PLGrid: The National Cloud Infrastructure PLGrid for EOSC – PLGrid ICON, which aims to build a modern cloud infrastructure enabling research and development work in accordance with the Open Science paradigm. We also care for its development by actively supporting the expansion of the EOSC environment and improving so-called Digital Twins, including in medicine and Earth sciences.

You can read about these and many other Cyfronet activities on the following pages of this publication, to which I warmly invite you. At the same time, I would like to thank all friends and users of Cyfronet for their cooperation and valuable feedback on the further development of the Centre.

Yours sincerely,

Marek Magryś
Acting Director
ACC Cyfronet AGH

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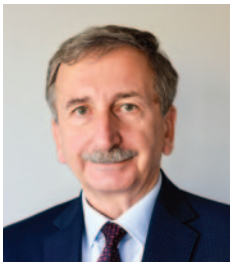

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The Academic Computer Center CYFRONET AGH is the longest-operating and one of the largest supercomputing and networking centres in Poland, with a history of providing access to supercomputing resources dating back to 1975.

For years, ACC Cyfronet AGH has been the operator of the fastest supercomputers in Poland, repeatedly listed on the TOP500 world list, as well as very high-capacity data storage systems. It has three data centres, its own fibre-optic network, as well as technical facilities, personnel and competencies, allowing it to operate 24 hours a day, 365 days a year. The centre is an administrator of the MAN network in Krakow and is an essential node of the PIONIER academic network, connected to the European GÉANT network.

Cyfronet is the organiser and leader of the PLGrid Consortium, consolidating national computing resources and providing a range of unique computing and IT support services for science, as well as the leader of the National Competence Center in HPC, which acts as a contact and access point for HPC for both academia and innovative entities in the economy and public administration.

ACC Cyfronet AGH plays a coordinating role in the projects included in the Polish Research Infrastructure Map (PMIB): National Supercomputing Infrastructure for EuroHPC and PLGrid National Cloud Infrastructure for EOSC. It is also a member of consortia implementing programs listed on the PMIB: CTA, EPOS, KMD, PIONIER-LAB, PRACE and Virgo, and additionally provides the computing infrastructure of High-Performance Computers along with the resources of storage systems and the computing infrastructure of the Metropolitan Area Network in Krakow (MAN) for conducting research work in other PMIB projects.

Cyfronet is actively involved in leading European projects related to the development of supercomputing technologies and services based on them, including WLCG (The Worldwide LHC Computing Grid), EGI (Advanced Computing Services for Research), PRACE (Partnership for Advanced Computing in Europe), EuroHPC JU (The European High Performance Computing Joint Undertaking), EOSC (European Open Science Cloud), EPOS (European Plate Observing System), LUMI (The Large Unified Modern Infrastructure), LUMI AI, LUMI-Q, Digital Twins in Earth and Health Sciences.

At the same time, Cyfronet participates in many other national and international research and development projects, which use both hardware resources and unique experience in building and developing integrated service platforms for scientific users. The Laboratories operating at Cyfronet bring together specialists who develop IT tools to support the development of science and technology, including modern medical diagnostics and therapy.

The centre also works with SMEs and large companies to enable the effective implementation of HPC (High-Performance Computing) and AI (Artificial Intelligence) in logistics, medicine, satellite image processing, CFD, drug research and the automotive industry.

An important aspect of Cyfronet's activities is the organisation of scientific events and specialised training and workshops related to HPC.

ISO 27001:2023 certificate

Under an audit conducted by the Polish Center for Testing and Certification S. A., on December 30, 2024, the Academic Computer Centre CYFRONET AGH received a certificate of compliance with the PN-EN ISO/IEC 27001:2023-08 (ISO 27001) standard.

The certificate confirms compliance with the requirements of the standard in the following scope:

1. services:
    - data processing and storage,
    - HPC,
    - cloud computing,
    - artificial intelligence,
    - colocation and data centre,
    - cyber security,
    - networking,
    - data transmission,
2. software development,
3. security audits,
4. IT training and consulting.

ACC Cyfronet AGH is certified in accordance with ISO 27001:2023

The awarding of the certificate is a confirmation that ACC Cyfronet AGH meets the high requirements of international standards.


IQNET

Building trust, together

Certificate

PCBC has issued an IQNet recognized certificate that the organization:

Academic Computer Center
CYFRONET AGH
ul. Nawojki 11, 30-950 Krakow, Poland

has implemented and maintains an

Information Security Management System

for the following scope:

- services: data processing and storage, HPC, cloud computing, artificial intelligence, colocation and data centre, cyber security, networking, data transmission;
- software development, security audits, IT training and consulting

which fulfils the requirements of the following standard:

PN-EN ISO/IEC 27001:2023-08

Issued on: 30.12.2024
Expires on: 29.12.2027

Registration Number: PL - I - 53/1/2024

Alex Stoichitoiu
President of IQNET

PCBC


POLSKIE CENTRUM BADAŃ I CERTYFIKACJI

CERTYFIKAT

Nr I - 53/1/2024

Akademickie Centrum Komputerowe
CYFRONET AGH
ul. Nawojki 11, 30-950 Kraków

spełnia wymagania

PN-EN ISO/IEC 27001:2023-08

w następującym zakresie:

- usługi: przetwarzania i składowania danych, HPC, chmury obliczeniowej, sztucznej inteligencji, kolokacji i centrum danych, cyberbezpieczeństwa, sieciowe, transmisji danych;
- wytwarzanie oprogramowania, audyty bezpieczeństwa, szkolenia i konsulting IT

Certyfikat pozostaje w mocy pod warunkiem przestrzegania przez Organizację wymogów powyższej normy.

Okres ważności certyfikatu:

od 30.12.2024 do 29.12.2027

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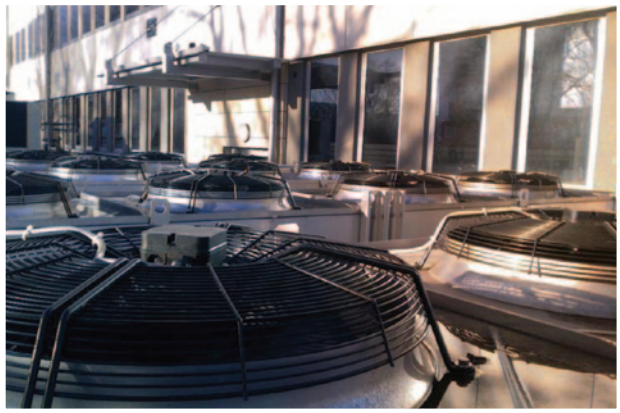
Polskie Centrum Badań i Certyfikacji S.A.



Helios – a new light for innovation in Polish science and economy

The Helios supercomputer is a system installed at ACC Cyfronet AGH, created as a result of work performed in the National Supercomputing Infrastructure for EuroHPC - EuroHPC PL project coordinated by Cyfronet. The supercomputer was built according to Cyfronet's design by Hewlett-Packard Enterprise based on the HPE Cray EX4000 platform. It consists of three computing partitions:

- CPU equipped with 75,264 AMD Zen4 computing cores and 200 TB of DDR5 RAM,
- GPU equipped with 440 NVIDIA Grace Hopper GH200 superchips,
- INT for interactive work, equipped with 24 NVIDIA H100 accelerators and fast local NVMe memory.

Helios achieves the theoretical computing power of 35 PFlops.

Helios in numbers	
Number of computing cores	75 264
Number of GPGPUs	464
Computing power	35 PFlops
TOP500 – the list of the world's fastest computers (November 2024 edition)	69th position (the GPU partition)
Green500 – the list of the world's most energy-efficient computers (November 2024 edition)	7th position (the GPU partition)

Helios' computing power for AI computing is almost 1.8 ExaFlops.

The Helios disk subsystem consists of two types of Lustre file systems: *scratch* with a capacity of 1.5 PB and a speed of over 1.8 TB/s and *project* with a capacity of 16 PB and a speed of almost 200 GB/s. All supercomputer components are connected via the Slingshot network with a speed of 200 Gb/s. Thanks to direct liquid cooling of the CPU and GPU partitions, it is possible to achieve a very low PUE (Power Usage Effectiveness) for the system, increasing its energy efficiency and reducing operating costs. Additionally, thanks to the recovery of waste heat produced by Helios, it will be possible to use it for heating.


HPE Cray
HELIOS

Athena – strong support for scientific calculations

Athena achieves the theoretical computing power of over **7.7 PFlops**. The accelerated computing system, installed in Cyfronet in 2021, provides the Polish scientific community with the computing resources based on the latest generation GPGPU processors and accelerators, along with the necessary data storage subsystem based on very fast flash memories.

Athena's configuration includes 48 servers with AMD EPYC processors and 1 TB of RAM (6,144 CPU compute cores in total), as well as 384 NVIDIA A100 GPGPU cards.

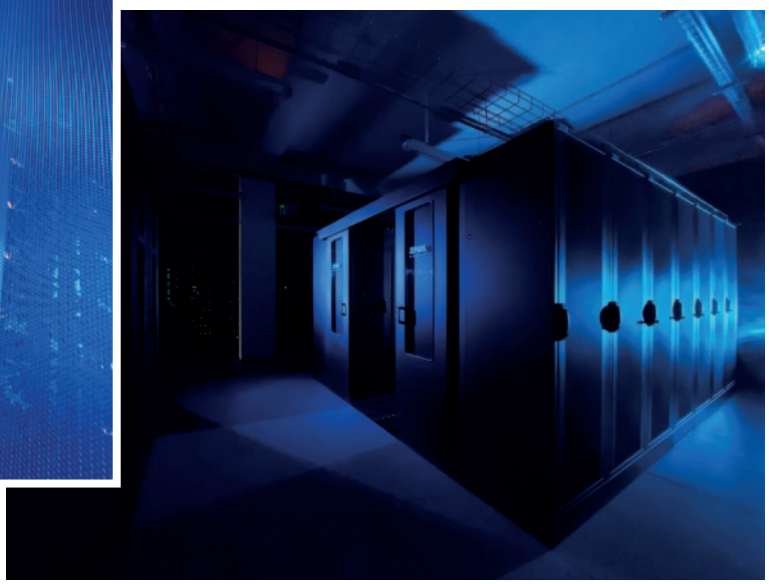
Athena in numbers	
Number of computing cores	6 144
Number of GPGPUs	384
Computing power	7.7 PFlops
TOP500 – the list of the world's fastest computers (November 2024 edition)	212th position

The indispensable element enabling the effective use of such high computing power is the provision of a high-performance internal network of a supercomputer (Infiniband HDR with 4x200 Gb/s bandwidth per server) and a very fast disk subsystem. It is built on the basis of the Lustre open-source software, currently used in Ares and Prometheus supercomputers, and dedicated disk servers equipped with flash memory in the NVMe standard. The system was installed in the existing Cyfronet data centre and integrated with the PLGrid infrastructure.

This type of infrastructure meets the needs of users of Cyfronet supercomputers, who use the computing infrastructure both to perform standard high-performance scientific simulations (HPC) and to apply artificial intelligence (AI) and machine learning (ML) methods to conduct research in the field of medicine, pharmacology, biology, chemistry, physics and many other fields of science. **Athena's computing power for AI computing is over 240 PFlops!**

The expected effect of delivering specialised computational resources of Athena will be the extension of the scope of research works, the possibility of undertaking advanced simulations and analyses, and increasing the possibilities of processing continuously flowing data from laboratories worldwide. The direct expected results of the work will be articles, scientific studies, patents, and, in the long term, innovative solutions that may be the basis for the development of new solutions in the economy.


ATHENA
ATHENA
ZPAS
GROUP
AGH



Ares – towards shorter computation time

In 2021, the Ares supercomputer was launched in Cyfronet. It is built of computing servers with Intel Xeon Platinum processors, divided into three groups:

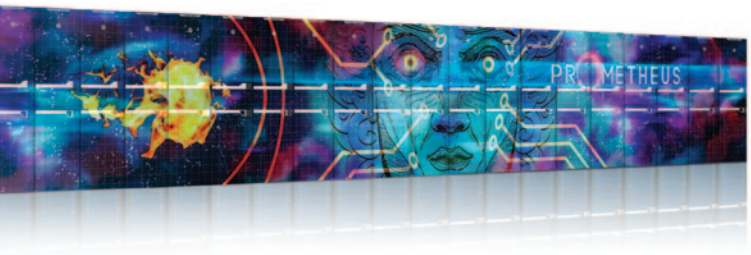
- 532 servers, each equipped with 192 GB of RAM,
- 256 servers, each equipped with 384 GB of RAM,
- 9 servers, each with 8 NVIDIA Tesla V100 cards.

Ares in numbers	
Number of computing cores	37 824
RAM	147.7 TB
Number of GPGPUs	72
Computing power	4 PFlops
TOP500 – the list of the world's fastest computers (November 2024 edition)	490th position

The total theoretical performance of the CPU parts is over 3.5 PFlops, and the GPU part is over 500 TFlops. Ares is supported by a disk system with a capacity of over 11 PB. An InfiniBand EDR network is used for data transfer. The supercomputer has 37,824 computing cores and 147.7 TB of RAM. It is also equipped with a liquid cooling system.

Ares complements Cyfronet's computing resources by providing a newer generation of processors and servers with more memory. It enables shortening the computation time of scientific tasks and addressing problems that so far could not be run on a large scale due to insufficient memory. In addition, placing Ares in Data Center Podole, a geographically different location than Helios, guarantees the continuity of the provision of computing services in crises.

Prometheus – PetaFlops computing power

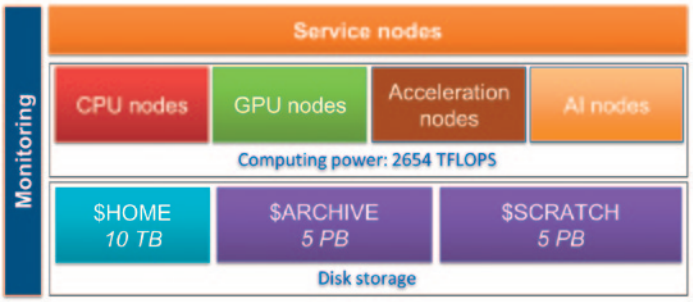


Prometheus consists of more than 2,239 servers based on the HP Apollo 8000 platform, combined with the super-fast InfiniBand FDR network with 56 Gbit/s capacity. Its energy saving and high-performance Intel Haswell and Intel Skylake processors offer 53,748 cores. These are accompanied by 283.5 TB of DDR4 RAM and by two storage file systems of 10 PB total capacity, and 180 GB/s access speed. Prometheus has also been equipped with 144 NVIDIA Tesla K40 XL and 32 NVIDIA Tesla V100 GPGPUs. The theoretical performance of Prometheus is 2.7 PFlops!

Prometheus in numbers	
Number of computing cores	53 748
RAM	283.5 TB
Number of GPGPUs	176
Computing power	2.7 PFlops

Due to the innovative technology of direct liquid cooling of processors and RAM modules, Prometheus is also one of the most energy-efficient computers in its class in the world. This was achieved by using the cooling water having a temperature of 28°C. To cool down the water to such a temperature in our climate it is enough to use cheap in use dry-coolers, instead of ice water generators, consuming relatively large amounts of electricity. With use of water cooling, electronic components operate at temperatures lower than normal, what positively affects not only the failure, but also allows to reach efficiency more than 5% higher than for a similar installation based on the classic air cooling. Furthermore, liquid cooling allowed for extremely high installation density of 144 computing servers in one rack, therefore Prometheus, weighing of more than 40 tons, covers 18 m^2 area and is placed on 20 racks only. This also has a significant impact on internal data transmission, because distances of connections are critical here.

Prometheus architecture



Prometheus has been installed in a high-tech computing room, exclusively adapted for its operation. The supercomputer's proper functioning is additionally supported by the accompanying infrastructure, including such systems as guaranteed power supply with an additional generator, modern air-conditioning and gas extinguishing.

Since its installation in 2015, Prometheus has been continuously listed (15 times) on the TOP500 list, occupying high places, with **38** – the highest noted spot. Prometheus was the fastest supercomputer in Poland 11 times.

Thanks to Prometheus users have received more than seven times greater opportunities compared to the previously used Zeus. Much more efficient processors, faster network of internal connections, and a greater amount of memory of Prometheus enable to perform calculations on a scale impossible to achieve using previous Cyfronet's resources.

Future technology cluster Faeton

Faeton reaches 288 TFlops of computing power. It consists of 64 compute servers, each equipped with two Intel Xeon Platinum 8352s processors supporting application memory encryption, 1 TB of RAM, and 100 Gbps Ethernet low-latency network adapters. In addition, the four compute servers are equipped with 8 TB of Intel Optane SCM memory. Faeton also includes service servers and 12 disk servers, offering more than 1 PB of NVMe disk storage and 12 TB of SCM memory. This configuration provides an excellent environment for developing innovative software, especially in data analytics (data science) and running applications in a high-performance, high-security cloud environment.

Faeton will be used to verify the applicability of new technologies, especially SCM (Storage Class Memory) in computing applications. The installation of such a system will enable work on the application of future technologies in the applications of Polish scientists and enterprises, giving them a competitive advantage by providing a platform using solutions at an early stage of development with a high innovation potential.

Four supercomputers from Cyfronet together on the TOP500 list of the fastest supercomputers in the world


TOP500 CERTIFICATE
The List.
Helios GPU - HPE Cray EX254n, NVIDIA Grace 72C 3.1GHz, NVIDIA GH200 Superchip, Slingshot-11
Cyfronet, Poland
is ranked
among the World's TOP500 Supercomputers
in the 63rd TOP500 List published at the ISC24 Conference on June 01, 2024.
Congratulations from the TOP500 Editors

In 2024, for the first time in history, the TOP500 list (the June edition) simultaneously included four supercomputers from one Polish computing centre. These were those operating in Cyfronet: Helios GPU (55th place), Athena (177), Helios CPU (305), and Ares (442). This success was repeated in November 2024, when the same four computers re-appeared on the TOP500 list, taking 69th, 212th, 348th and 490th place, respectively.

The story of the machines installed in Cyfronet that were on the TOP500 list began in 1996 when the SPP1200/XA-32 computer took 408th place. After a long time without records, the Zeus supercomputer appeared on the list in 2010 and remained there until 2015. From then on, until 2022, Cyfronet has been represented by Prometheus, which was joined by Ares in June 2021, Athena in June 2022, and Helios in November 2023.

Zeus supercomputer

- 2010 - VI, 161st place, 55 Tlops
- 2010 - XI, 85th place, 105 TFlops
- 2011 - VI, **80th** place, 124 TFlops
- 2011 - XI, 88th place, 162 TFlops
- 2012 - VI, 89th place, 271 TFlops
- 2012 - XI, 106th place, 357 TFlops
- 2013 - VI, 114th place, 374 TFlops
- 2013 - XI, 146th place, 374 TFlops
- 2014 - VI, 176th place, 374 TFlops
- 2014 - XI, 211th place, 374 TFlops

Prometheus and Zeus supercomputers

- 2015 - VII, 49th and 269th place, 1659+374 TFlops
- 2015 - XI, **38th** and 387th place, 2399+374 TFlops

Prometheus supercomputer

- 2016 - VI, 49th place, 2399 TFlops
- 2016 - XI, 60th place, 2399 TFlops
- 2017 - VI, 72nd place, 2399 TFlops
- 2017 - XI, 78th place, 2399 TFlops
- 2018 - VI, 103rd place, 2399 TFlops
- 2018 - XI, 131st place, 2399 TFlops
- 2019 - VI, 174th place, 2399 TFlops
- 2019 - XI, 241st place, 2399 TFlops
- 2020 - VI, 288th place, 2399 TFlops
- 2020 - XI, 324th place, 2399 TFlops

Ares and Prometheus supercomputers

- 2021 - VI, **216th** and 373rd place, 3510+2399 TFlops
- 2021 - XI, 267th and 440th place, 3510+2399 TFlops

Athena, Ares, and Prometheus supercomputers

- 2022 - VI, **105th**, 290th and 475th place, 7709+3510+2399 TFlops

Athena and Ares supercomputers

- 2022 - XI, 113th and 323rd place, 7709+3510 TFlops
- 2023 - VI, 123rd and 362nd place, 7709+3510 TFlops

Athena, Helios CPU, and Ares supercomputers

- 2023 - XI, 154th, **290th** and 403rd place, 7709+3400+3510 TFlops

Helios GPU, Athena, Helios CPU, and Ares supercomputers

- 2024 - VI, **55th**, 177th, 305th and 442nd place, 30.44+7.71+3.35+3.51 PFlops
- 2024 - XI, 69th, 212th, 348th and 490th place, 30.44+7.71+3.35+3.51 PFlops

Supercomputers from Cyfronet on the TOP500 list

The world's top energy efficiency

In 2024, four of Cyfronet's supercomputers that took place on the TOP500 list have also been ranked on the Green500 list of the most ecological supercomputers. The main criterion (energy efficiency) is calculated as the ratio of the number of floating-point operations per second (computing power of a supercomputer) to energy consumption: Gflops/W. Helios GPU partition's **3rd place** in the June edition and 7th place in the November edition of the Green500 list was a particular success. This means Helios became the most energy-efficient supercomputer from the top hundred of the TOP500 list. This position proves an excellent ratio of the provided computing power to the electricity consumption. So high energy efficiency means Helios offers more computing power for each kilowatt-hour consumed than less efficient systems. Hence, calculations using Helios are cheaper than those using other machines and have a smaller environmental impact. In 2024, the remaining supercomputers from Cyfronet – Athena, Helios CPU, and Ares – were also listed on the Green500 list and took 32nd, 95th, and 129th place in the June edition, and 53th, 113th and 145th place in the November edition, respectively.

Supercomputers usage

Supercomputers in Cyfronet are part of the European cloud and grid infrastructure under the European Grid Infrastructure (EGI). At the same time, they are also important supercomputers in the PLGrid nationwide computing infrastructure – the platform for conducting *in silico* research and enabling calculations with the use of high-performance computers, also within the cloud and grid architecture.

Scientists can access the supercomputers' resources via the PLGrid infrastructure. Dedicated computing environments and specialised IT platforms enable the conduction of increasingly complex research problems. The research portfolio carried out with the help of Cyfronet supercomputers is quite reach. It includes:

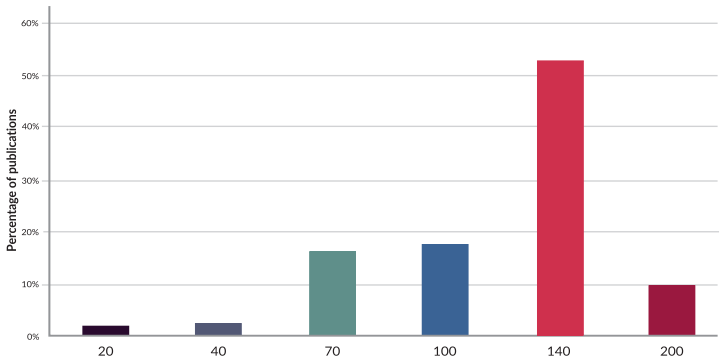
- testing the spectral properties of chemical compounds,
- development of artificial intelligence models for segmentation of lesions on CT images of the lungs and MRI of the liver,
- pedestrian detection based on the signal from the event camera, using quantized neural networks,
- prediction of gravitational waves using machine learning,
- modeling of phase separation of proteins and polypeptides,
- analysis of meteorological data using machine learning,
- modeling the properties of polymers and nanomaterials,
- molecular dynamics simulations of electrolytes,
- the use of artificial intelligence to support the diagnostic process in veterinary medicine.

A wide range of research topics is evidence of a constantly increasing number of scientists aware of supercomputers' advantages. With their help, one can get the final results of massive simulations many, many times faster compared to the case of an ordinary desktop computer. Supercomputers can significantly reduce the time of computations that using a single computer would often take many years. Here, they may be usually performed within a few days. What is essential is that Cyfronet users can benefit from professional support – from complete documentation through training to individual consultations with experts.

In addition to individual scientists and small research groups, even international consortia carry out calculations from many different scientific disciplines with the help of supercomputers – of course, with the participation of Polish scientists. Scientific computations do not include simulations only. Computing power is utilised by Polish researchers also within international scientific projects, including experiments like CTA, LOFAR, EPOS, Large Hadron Collider in CERN and the gravitational waves in LIGO and VIRGO detectors.

Year	No. of jobs	CPU time in years
Cyfronet supercomputers		
2008	603 525	207
2009	2 227 804	876
2010	4 009 049	990
2011	7 557 817	5 052
2012	8 126 522	7 923
2013	7 932 978	11 016
2014	7 694 224	12 980
2015	7 505 763	15 952
2016	7 748 677	24 653
2017	9 066 892	39 232
2018	8 342 686	42 436
2019	4 993 639	44 027
2020	5 696 919	41 761
2021	5 549 582	43 409
2022	6 227 244	48 716
2023	11 468 532	52 722

Ministry marks of articles published in 2023 by Cyfronet Users in scientific journals



Obviously, even the highest positions in the TOP500 list, or the latest technologies used to build high-performance computers do not fully reflect the importance of this kind of computing resources for the Polish scientific community. The usefulness of supercomputers provided by ACC Cyfronet AGH as a tool for conducting research is best evidenced by statistical data on their use.

The table presents the aggregated key data on the number of computational tasks and their duration, performed by Cyfronet for other units.

It is worth mentioning that huge users' demands for computing power and space for data storage would not be fulfilled without continuous extension of computing resources and disk storage. Therefore, we carefully analyze users' suggestions and statistical data related to carrying out computations together with the world's trends in computing.

The scientific level of the tasks carried out with the use of the infrastructure provided by ACC Cyfronet AGH is very high. This is evidenced by the results of scientific and research works carried out in 2023 using this infrastructure, which were presented in many publications.

Comprehensive infrastructure of efficient and safe storage of digital data

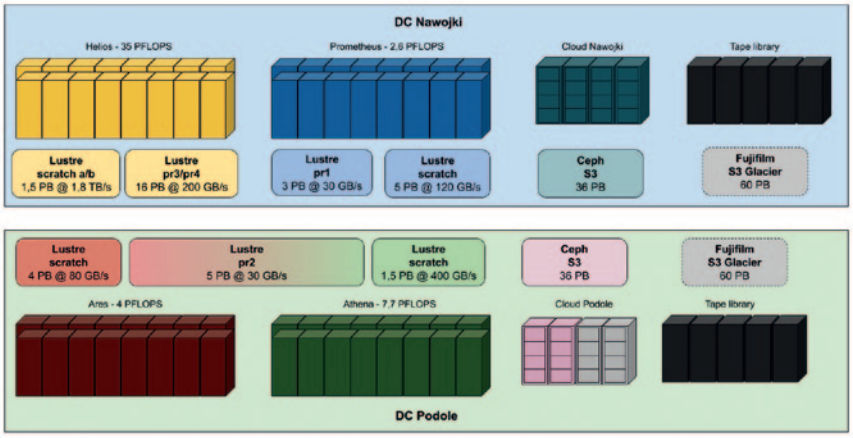
The currently observed phenomenon of the rapidly growing amount of digital information also applies to the scientific community. Access to very efficient supercomputers enables the analysis of large-scale research problems, generating huge data sets. They require a completely new approach to information processing and storage. This problem, being currently one of the most important challenges of the modern digital world, is described by the concept of BigData. Also, in ACC Cyfronet AGH, the growing expectations concerning available capacity, speed, and additional functionalities of storage resources are visible because of the provision of more efficient computing systems. The architecture of the Cyfronet Data Storage System, the main mass storage platform for High-Performance Computers, is composed of the following elements:

- the SAN network – the efficient and highly available network dedicated to communication among devices within the Data Storage System, and clients using shared resources or services,
- disk arrays and servers of various types, offering the storage space for the users' data – starting from fast, but expensive and less capacious solutions, and ending with the devices with large storage capacity and relatively cheap, but with lower efficiency,
- service servers, with specialised tools and virtualisation software, providing users with functionalities such as automatic backup and archival, hierarchical data storage systems, high-performance hardware file platforms or distributed network file systems,
- tape libraries and specialised software used to store critical user data on magnetic media,
- additional infrastructure, including Ethernet, Infiniband as well as solutions supporting IT infrastructure management and enabling secure magnetic media storage.

The total storage capacity of Cyfronet disk and tape resources currently exceeds **270 PB**.

Mass storage for supercomputers

The proper teaming of computing infrastructure with the right selection of storage solutions can assure the best quality of services provided to scientific users. The scale of problems in this area grows with the complexity and efficiency of the supercomputers used. Currently, data storage systems attached to Cyfronet supercomputers store billions of files up to terabytes. The broad thematic scope of research on the resources provided by Cyfronet is reflected in the variety of configurations of the Centre's key supercomputers and, thus, in the structure of dedicated storage resources. Cyfronet's data storage system resources are placed in two locations.



Supercomputers use, among others, efficient temporary space, the so-called scratch. The critical element here is the speed of operation, which is why it is based on a high-speed distributed file system architecture – Lustre. The advantage of Lustre is the ability to scale the capacity and efficiency of the disk space. By combining the capacity of multiple servers, I/O bandwidth is aggregated and scales with additional servers. Moreover, bandwidth and/or capacity can be easily increased by dynamically adding more servers without interrupting users' computations. Currently, all supercomputers in Cyfronet use the scratch space implemented by Lustre. In the case of Prometheus, this space has a capacity of 5 PB and a speed of 120 GB/s. Ares has the space with a total of 4 PB and a speed of 80 GB/s. In both of these computers, the scratch space is realized with the help of mechanical disks. In the case of Athena and Helios, user data is stored on solid-state drives. Using this type of solution significantly increases the system's efficiency. The capacity of this type of space for Athena is 1.5 PB and achieves a bandwidth of 400 GB/s. In the case of Helios, the scratch space has a capacity of 1.5 PB and a speed of 1.8 TB/s.

Most of Cyfronet's disk memory resources are dedicated to the needs of users of domain services developed in the PLGrid program. The PLGrid infrastructure offers a dedicated workspace for groups using domain services – the functionality necessary to enable collaboration between scientists working in geographically dispersed locations. This functionality is implemented using the Lustre file system. The maximum capacity of the /pr1 resource in the Prometheus supercomputer is 5 PB, and the total speed of reading and writing operations reaches 30 GB/s. In the case of Ares and Athena, the /pr2 resource has the capacity of 5 PB and the speed of 30 GB/s. In the case of Ares and Athena, the */pr2* resource has a capacity of 5 PB and a speed of 30 GB/s. In the case of Helios, the */pr3 and /pr4* resources have a capacity of 16 PB and a speed of 200 GB/s.

The object-oriented data storage system is an additional resource for storing users and projects' data in Cyfronet. It is based on the CEPH software. The data in this system is available through the S3 protocol based on the REST API and is stored in globally unique containers (buckets) in which users store their data in the form of objects.

A particular case of mass storage are resources for large projects and international collaborations in which Cyfronet participates, such as WLCG (Worldwide LHC Computing Grid), analyzing data from the LHC detector at CERN, or CTA (Cherenkov Telescope Array), studying gamma radiation using a network of radio telescopes. These projects require substantial disk resources, often available using unusual protocols such as SRM, xroot, or GridFTP. Cyfronet provides this type of disk space using several instances of dedicated DPM software (Disk Pool Manager) and using dedicated networks such as LHCone. The total capacity of DPM systems in Cyfronet exceeds 2 PB.

Currently, the total available disk capacity used by ACC Cyfronet AGH is approximately **150 PB.**

Backup-archiving services in detail

ACC Cyfronet AGH provides its users with a wide portfolio of services related to securing information stored in a digital form. In addition to advanced technological solutions such as communication networks dedicated to storage systems, modern disk arrays or hardware file servers, the Centre also performs conventional backup-archiving services, based on magnetic media. Contrary to the expectations of the inevitable end of solutions using data storage on magnetic tapes, this technology is constantly evolving, and offers in successive generations not only the increasing capacity of the media, but also significantly better capacities and mechanisms supporting the safety and effectiveness of the information storage (e.g. data encrypting and compressing algorithms, which are embedded in the tape drives).

Cyfronet has three tape libraries with over 9 thousand slots for LTO magnetic tape drives and 44 drives of the VI, VII and IX generations. A single LTO-9 magnetic medium has a physical capacity of 18 TB and allows recording at a speed of up to 400 MB/s. Described resources are used for performing current backup and archive of essential information resources of the Centre's users.

Backup is performed on the active data that might be currently in use through a replication process from the source location to a separate, isolated destination. The ideal backup procedure ensures consistency of the source and backup data, both at the level of a single object (a file located on a hard drive) and in the case of complex IT systems, such as databases or mail servers, as well as virtual environments. Physically, the cloning process is usually done by copying the source data from the backup client disk to disk/tape resources of the target backup server, using a dedicated or shared access medium, such as Ethernet or SAN. An archive aims to ensure the security of unused data and release occupied storage resources. In contrast to the backup, the archive is performed once by the migration of the data from the source location to the destination.

ACC Cyfronet AGH provides a wide range of backup services, addressed directly to users, and operating without their interaction. Among those at users' disposal are those based on FTP, NFS, and SCP network protocols that act within the dedicated backup servers. These machines provide backup solutions for users, allowing them direct access to the backup data. It is up to users to decide which data they treat as a backup and which as archives.

The total storage capacity of Cyfronet tape resources currently exceeds **120 PB**.

PLGrid – advanced computing solutions for Polish science and economy

PLGrid is a state-of-the-art computing infrastructure coordinated by ACC Cyfronet AGH, which was built and developed to support the Polish sectors of science, economy, and public administration. Its advanced supercomputing, quantum and cloud resources enable research and development at the highest global level, supporting innovation and development of new technologies in many areas of science and economy.

The PLGrid Consortium

The origins of the PLGrid infrastructure date back to January 2007, when the PLGrid Consortium was established on the initiative of ACC Cyfronet AGH. It includes Poland's largest computing centres:

- Academic Computer Centre CYFRONET AGH in Krakow (the Consortium leader),
- Centre of Informatics Tricity Academic Supercomputer and networK GUT in Gdansk,
- Interdisciplinary Centre for Mathematical and Computational Modelling UW in Warsaw,
- National Centre for Nuclear Research in Świerk (from 2019),
- Poznan Supercomputing and Networking Center IBCh PAS in Poznan,
- Wroclaw Centre for Networking and Supercomputing WUST in Wroclaw.

The infrastructure was built in a series of PLGrid projects (PL-Grid, PLGrid Plus, PLGrid NG, PLGrid Core). The original goal was to provide Polish scientists with modern IT tools and services based on supercomputing resources. In 2009-2012, a national grid infrastructure was created to support scientific research carried out by geographically dispersed teams. Since 2011, specialised tools and services for various scientific fields have been developed.

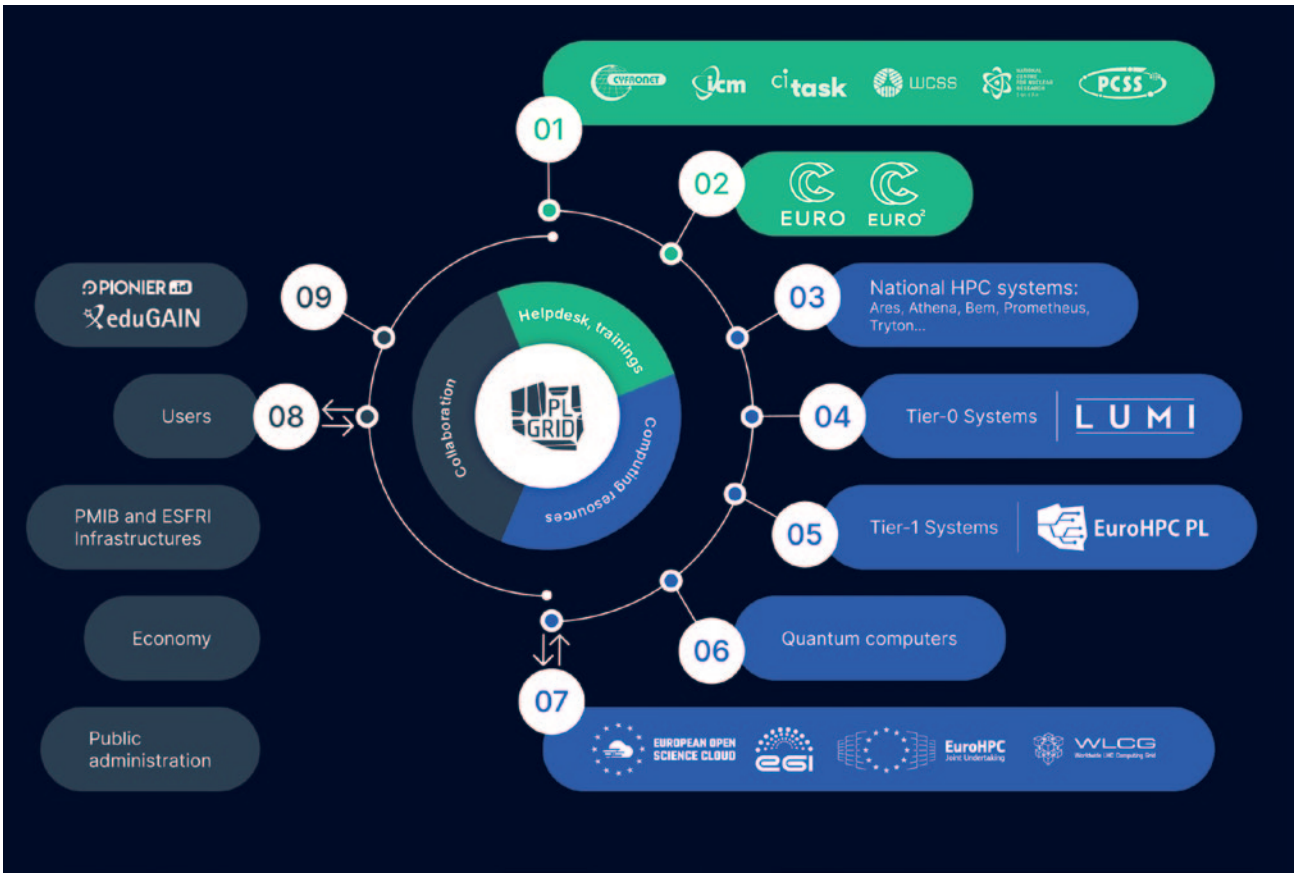
Following the expansion of the PLGrid's national computing infrastructure in 2014, also made possible by its integration with the European infrastructure within the EGI organisation of computing and storage resource providers, PLGrid users gained access to cloud computing and new tools to support computing on big data, among other things. New dedicated computing services were also implemented in the following years for research groups from various scientific disciplines, identified as priorities in the National Research Program.

Beginning in 2020, PLGrid has been conducting activities related to the EuroHPC JU, a European effort to develop an exascale computing infrastructure. Under the aegis of the EuroHPC JU, EuroHPC National Competence Centers have been established to provide access to world-class supercomputers and provide technological and training support for HPC, big data collection, storage, processing and analysis, and artificial intelligence.

Constant development

From 2023 to 2025, carrying out the tasks of the EuroCC 2 project, the identification and filling of competence deficits in the European EuroHPC infrastructure is being conducted. In Poland, access to European HPC resources has also been provided to users from the private and public sectors. Support for implementing HPC services in the field of artificial intelligence is being provided, and since 2023, PLGrid has offered its users access to a platform that allows computing with quantum accelerators.

The PLGrid National Cloud Infrastructure for EOSC - PLGrid ICON project was launched in 2024. The project aims to build a state-of-the-art cloud infrastructure to enable research and development in accordance with the Open Science paradigm. PLGrid ICON will be a part of the European Open Science Cloud (EOSC). The PLGrid ICON cloud will provide an environment for R&D work, with a particular focus on data science and artificial intelligence applications.



Fastest supercomputers in Poland and Europe

The PLGrid infrastructure offers access to all modern HPC resources belonging to ACC Cyfronet AGH (including Athena and Helios – the fastest machines in Poland) and supercomputers located in the computing centres of consortium members. In addition, ACC Cyfronet AGH represents Poland in the LUMI consortium, within the framework of which, thanks to the financial contribution of the state and the cooperation of our specialists, Polish scientists can use the resources of this fastest European supercomputer to conduct research based on large-scale computing, parallel processing of massive data sets and multifaceted analyses, including with the use of artificial intelligence.

Supercomputers provided in the PLGrid infrastructure have for years earned high, prestigious places on TOP500 lists – the fastest supercomputers and Green500 – the most energy-efficient supercomputers. It is worth noting that the June 2017 TOP500 list included 4 PLGrid supercomputers: Prometheus, Eagle, Triton, and Bem. On the other hand, in June 2024, the machines made available in PLGrid were ranked in 5 positions: Helios GPU, Lem, Athena, Ares and Helios CPU.

In turn, on the Green500 list in 2022, Athena was ranked 10th, and in 2024, Helios GPU was ranked 3rd.

Offer and benefits

Access to HPC means, for anyone doing scientific or economic computing, the possibility of accelerating computational processes many times over. This makes it possible to run complex simulations and analyses, even on massive data sets, in a much shorter time and on a much larger scale, which is now crucial in fields such as physics, chemistry, molecular biology or the manufacture of new materials. With their quantum resources and parallel processing of vast amounts of data, supercomputers also support the development of AI and ML algorithms as well as discoveries and innovations in big data.

PLGrid offers excellent computing power, cloud and disk resources, and access to numerous scientific software packages and world-class data storage services. Access to these resources is entirely free of charge for Polish scientists and all those engaged in scientific activities associated with a Polish university or research centre, including students and PhD students.

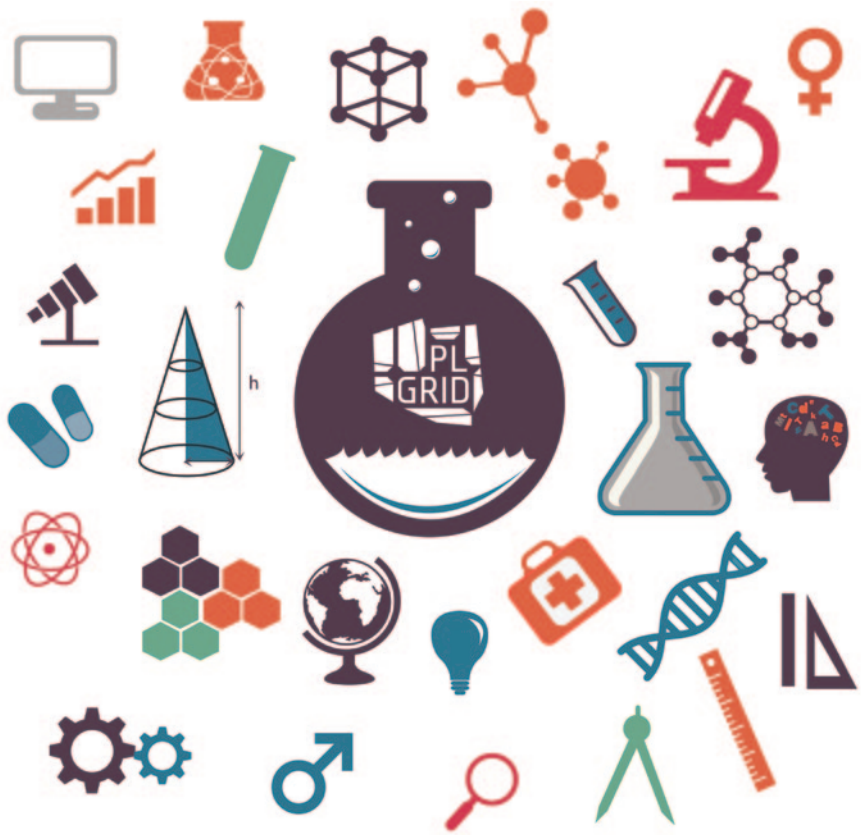
The infrastructure is not only the most modern computing machines in Europe but also people – and their expert knowledge. The cooperation with PLGrid provides comprehensive technical support through the continuous development of documentation and daily advice to PLGrid users by experts in the Helpdesk system. IT consulting and training are also offered.

To provide Users with convenient and intuitive use of resources, and based on modern technologies, the PLGrid Portal (***https://portal.plgrid.pl)*** was created. It enables a quick and secure application for

computational grants. An intuitive and user-friendly interface makes navigating and using our services easy, and the highest security standards protect Users' data and privacy.

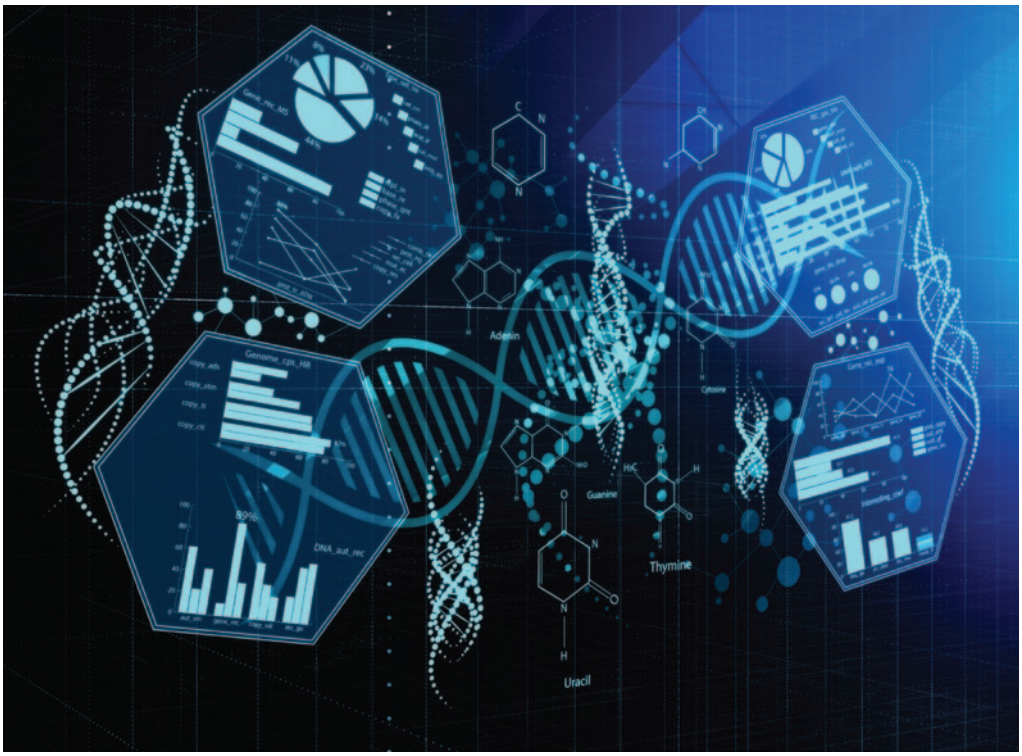
Daily support in calculations is also provided by a new, unified, more precise and continuously updated documentation – the PLGrid Guide, available at ***https://guide.plgrid.pl/en/***. Thanks to its simple navigation, you will find the information you need even faster.

For more advanced Users, there is also a Compendium of knowledge necessary to create more efficient applications, optimally utilising the computational capabilities of our computer systems (***https://kompendium.plgrid.pl/***).



Application examples

Access to state-of-the-art technologies significantly improves the quality and efficiency of ongoing research, resulting in nearly four thousand publications produced with PLGrid's participation. Among them, you can find many important and groundbreaking works in today's key fields of knowledge, including AI, medicine, and projects aimed at counteracting the effects of climate change on the Earth.



Artificial intelligence

Our users conduct much research on artificial intelligence algorithms and the possibility of their practical use. With the support of PLGrid, language models and natural language processing works are being developed.

Computing power in modern medicine

Scientists at the Sano Center for Computational Medicine (ACC Cyfronet AGH) use artificial intelligence, advanced bioinformatics algorithms and simulations to support doctors in the diagnostic and treatment process. State-of-the-art supercomputers make it possible to precisely select the most beneficial treatment for a given patient and speed up the development of new drugs, vaccines and medical procedures.

Weather and climate change

Thanks to supercomputers, Polish scientists are not only improving digital weather models for more accurate and verifiable weather forecasts but also assessing global climate change and conducting research to develop mitigating methods.

Reaching for the stars

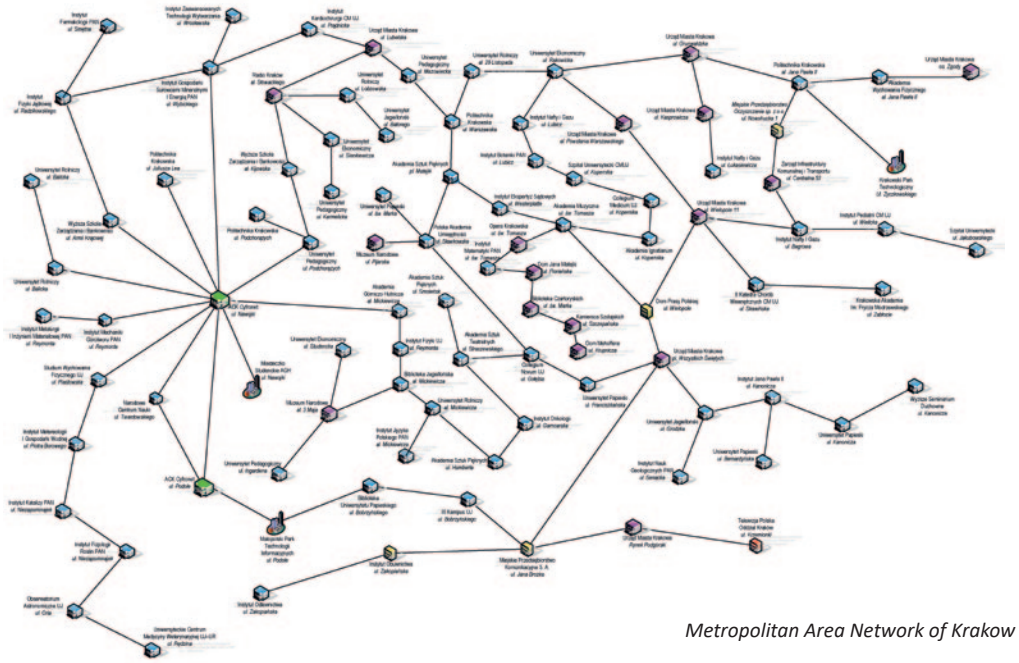
Modern astronomy instruments scan the sky daily, generating vast amounts of data, often counted in giga and terabytes. On the other hand, modelling astrophysical processes requires extensive resources and advanced computational methods. Polish astronomers are successfully using PLGrid to explore the mysteries of the universe.

Gain new opportunities with PLGrid

Joining PLGrid Users enables you to conduct world-class research using state-of-the-art IT tools with the support of a team of experts. Please visit ***https://www.plgrid.pl/***.

Metropolitan Area Network

One of the major characteristics of the present science is the complexity of research challenges, including their multidisciplinary character, use of heterogeneous models, resources and massive amount of data produced by a variety of sources. Research is not performed by a small group of scientists anymore, but by international consortia. Fast and reliable network connectivity is essential to bind those usually geographically distributed resources together. Therefore, one of the principal tasks of the ACC Cyfronet AGH is developing and maintaining the Metropolitan Area Network (MAN) to achieve its availability 24/7.



Metropolitan Area Network of Krakow

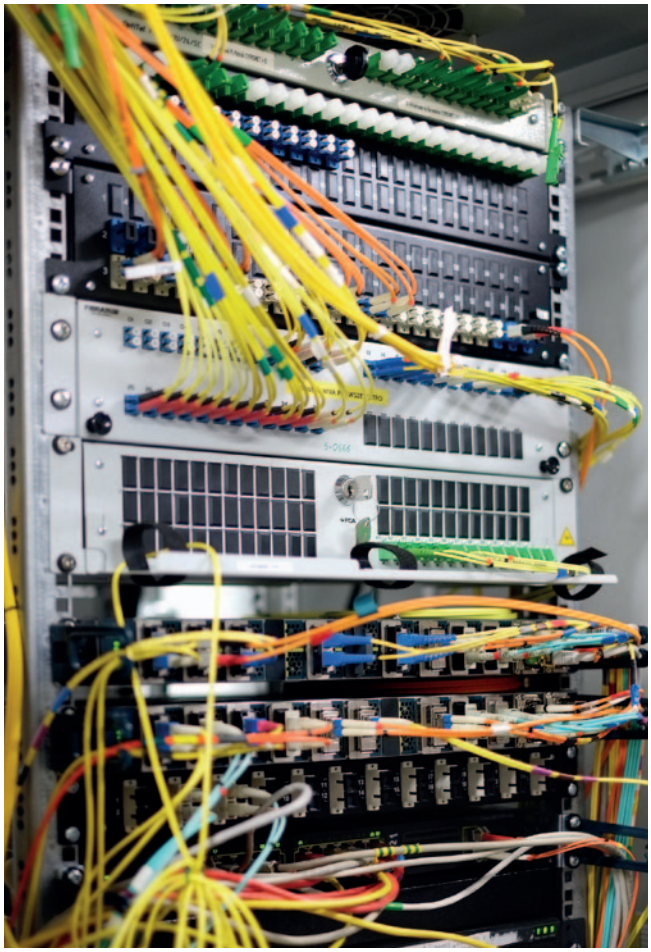
Main characteristics of MAN

It is impossible to attain high network availability without its continuous development and adjustment to users' needs. At present, the length of dedicated fibre-optic links reaches over 200 km. The core links of the network are located in the Old Town area and reach the academic campus of AGH University. Furthermore, the network also covers Bronowice, Krowodrza, Czyżyny and Nowa Huta zones. The recent expansion of the network included such distant research centres as Prokocim, Borek Fałęcki, Balice and the 3rd campus of the Jagiellonian University in Pychowice. Development of the core backbone also includes other directions, up to the borders of Kraków.

The fibre-optic infrastructure is the basis of the MAN operation. ACC Cyfronet AGH makes efforts to include in it the largest possible number of university facilities and research institutions. At the same time, due to the ever-growing role of modern communication means in everyday work, it is crucial that fibre-optic infrastructure, in addition to high bandwidth, could also ensure secure communication. It is realised through the use of backup links, which maintain the continuity of operation when primary routes are broken.

The core data link layers are implemented using top-quality equipment with 1 and 10 Gb Ethernet technologies, while 100 Gb interfaces are gradually being introduced. Additionally, the subnet was equipped with two switches with eight 100 Gb interfaces and sixteen 10 Gb interfaces. Each backbone network switch is connected with at least two (and sometimes with three) neighbours for automatic and transparent recovery in case any network device or link fails. Our users can obtain fibre-optic connectivity to the network via 10/100/1000 Mbps or 1 Gbps Ethernet cables and through traditional modem uplinks.

The Metropolitan Area Network is directly connected from Kraków to Warsaw, Katowice, Bielsko-Biała and Rzeszów through the PIONIER (Polish Optical Internet) network. Currently, the links can serve up to 2x10 Gbps capacity. High-Performance Computing centres in Poland (Gdańsk, Kraków, Poznań, Warsaw and Wrocław) are integrated with links of 2x100 Gbps capacity. The PIONIER network also enables communication with major national and foreign computing centres. International connectivity is achieved through the GEANT scientific network with 100 Mbps capacity. In addition, the reserve connection is established.



Network services provided to the users

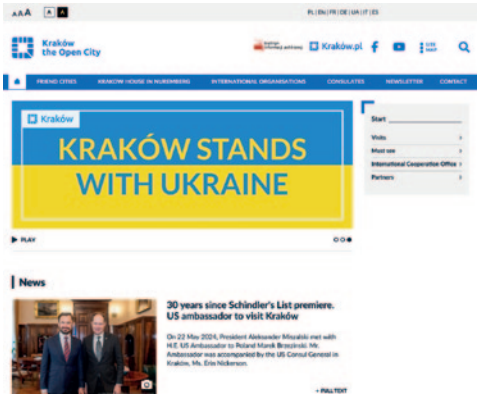
Since the beginning of the Polish Internet (mid-1991), ACC Cyfronet AGH has actively participated in developing telecommunications infrastructure and, what is very important, the wide range of Web services. Those include:

- **e-mail**: accessed via SMTP protocol or web interface *http://poczta.cyfronet.pl*,
- **www**: CYFRONET operates a set of web sites, which in addition to news from the world of science, present information on the culture and many other fields,
- **news**: discussion groups covering all areas of interest – from highly specialised scientific to general-purpose boards,
- **dns**: domain name system servers – performing translations of network domain names to IP addresses for users of the Krakow MAN,
- **ftp**: CYFRONET mirrors major international software archives, providing shareware and freeware applications for MS Windows and UNIX systems. The establishment of this service has significantly reduced the traffic on CYFRONET's international links while at the same time enabling faster downloads of software for users of the Krakow MAN,
- **eduroam**: provides the academic network access at all locations on eduroam in the world with a single authorised account,
- **box**: a network drive (*http://box.cyfronet.pl*) allowing file exchange and synchronisation. The drive can also be accessed from mobile devices via a dedicated application.

Network services in numbers in 2023	
Number of e-mails	> 19 000 000
Number of e-mail server sesions	> 54 000 000

Portals and mobile applications

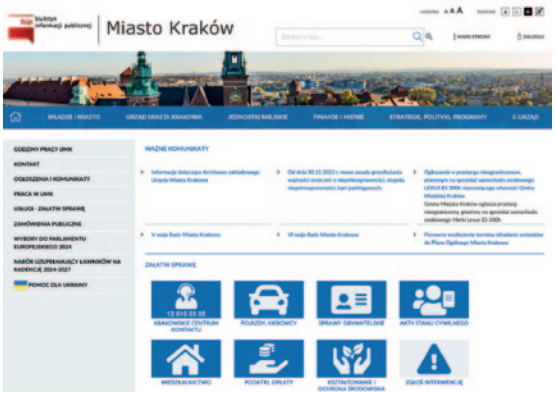
The Centre does not limit its activities to the scientific areas only – it also contributes to the development of the information society. The Web server at ACC Cyfronet AGH serves as an Internet hub for the entire Kraków scientific community. The Centre continues to develop and extend its Web portal, which has gained substantial popularity over the years. The *www.cyfronet.pl* website is fully adapted for viewing information on mobile devices.



Cooperation with the Kraków City Hall is important for the Centre. The agreement between the Municipality of Kraków and Cyfronet regarding the City promotion has resulted in the creation of an up-to-date portal. Aside from scientific information, the portal introduces its readers to the culture, historic sites, tourism, local transit and many other aspects of life in Kraków.

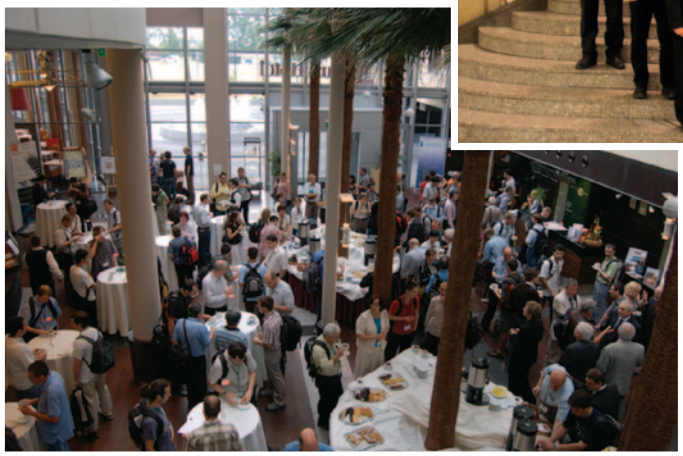
In collaboration with the City Hall, the Centre has been developing and running the Internet Bulletin for Public Information in the Kraków Region. The portal publishes the Public Information Bulletins of the Kraków City Hall and several hundred municipal institutions, libraries, schools, kindergartens, etc.

For many years, ACC Cyfronet AGH has been actively cooperating in creating the official website of Kraków, which functions as the Municipal Internet Platform „Magical Krakow" (MPI). MPI provides over 40 thematic portals, including the leading city portal, available at *www.krakow.pl*. Cooperation with the City Hall also explores the area of mobile devices. Cyfronet has developed – among others – a mobile application, "Kraków.pl". The app can be used as a Kraków city guide and a source of important information like phone numbers, info points, consulates, and pharmacies. Our app is available in a few languages.



MPI portals and the Kraków.pl web application have been repeatedly awarded and nominated, for example, for the World Summit Award as the best e-government service in Poland. Meanwhile, the mobile version of the portal was awarded at the Mobile Trends conference as the best mobile city website in Poland.

photo: AGH archive




Digital Infrastructures for Research 2010

IT services

ACC Cyfronet AGH provides a mature computing infrastructure for Polish science based on several main pillars. Furthermore, complex support and training are available for the users.

Computational resources

Helios, Athena, Ares and Prometheus supercomputers provide about 50 PFlops of the computing power

Storage

150 PB of disk and 120 PB of tape storage space together with fast scratch Lustre filesystems enable big data processing and analyses.

Professional IT solutions

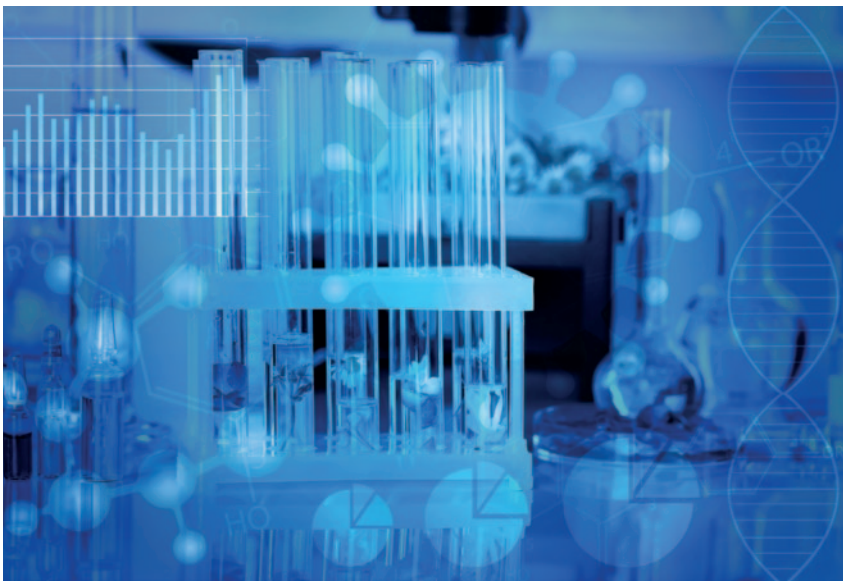
Cyfronet provides a number of advanced tools enabling easy access to distributed data sets and computational resources, their analysis, visualization and sharing.

Data center

Three Data Centers are a full guarantee of the security in the provision and maintenance of the IT infrastructure throughout the year, 24 hours a day, 7 days a week.

Advanced computing platforms and domain-specific services

Among the scientists conducting research with the use of high-performance computers and large storage resources there is a need for different types of interaction with a computer or with the infrastructure. To address these needs Cyfronet provides a number of advanced IT platforms and dedicated services that hide the complexity of the underlying IT infrastructure and, at the same time, provide the functionalities important from the point of view of scientists from the particular field, precisely tailored to their needs.



Together with computing infrastructure we provide a selection of tools, which enable researchers to perform complex, large-scale experiments and manage their results in an easy way. The efficiency of the performed analyses and the safety of their associated data are guaranteed by appropriate IT solutions, benefitting from the extensive experience of Cyfronet's developers. All those services are provisioned in the framework of the PLGrid infrastructure, allowing Polish scientists and their foreign collaborators to access it in a convenient manner.

Among others, at the Centre we offer advanced tools and graphical interfaces that enable the construction of dedicated environments for scientific research, building application portals, conducting virtual experiments, visualization of calculations' results, executing complex scenarios with parallel tasks, as well as supporting uniform and efficient access to data. All of these services are important support for researchers, as they have an impact on improving and, where possible, automating the work of research groups, which greatly accelerates obtaining research results. On subsequent pages, we will learn about the capabilities of selected services.

Invitation to cooperate

We are looking for people interested in the development of domain-specific services. We also offer support in scientific research.

We encourage scientists to send us their program codes for the compilation by the experts at the Centre. After installation, we provide assistance in their effective use. We also enable the use of scientific software licenses held by research groups.

ONEDATA

Onedata is a global data management system, which provides transparent access to data stored on distributed storage resource managed by multiple providers. Onedata can scale to meet the needs of small user communities or large federations of users and storage providers, making it a perfect solution for large research initiatives, long-tail of science as well as for commercial purposes. Onedata allows users to rely on a single solution for managing their personal as well as research data sets and access them efficiently on any machine, from personal laptop as well as from a Cloud virtual machine.

Onedata provides a unique federation system based on zones, which enables storage providers to organize into trusted federations and allows users to easily request storage resources from providers within a zone.

Features for users

- Unified access to data stored on heterogeneous storage systems distributed across the infrastructure. With Onedata, users can access their data from anywhere, as the system automatically replicates and transfers necessary blocks on demand.
- All data is organized into *space*, which can be regarded as virtual folders or volumes, accessible from any client machine via POSIX protocol.
- Easy to use web based Graphical User Interface for data access, discovery and management.
- Support for easy data sharing and collaboration with other users, while ensuring security through custom Access Control Lists and creation and management of user groups.

- Open data publishing functionality integrated into the user interface, enabling publication of prepared datasets, registration of DOI identifiers and indexing in open access portals.

Features for administrators

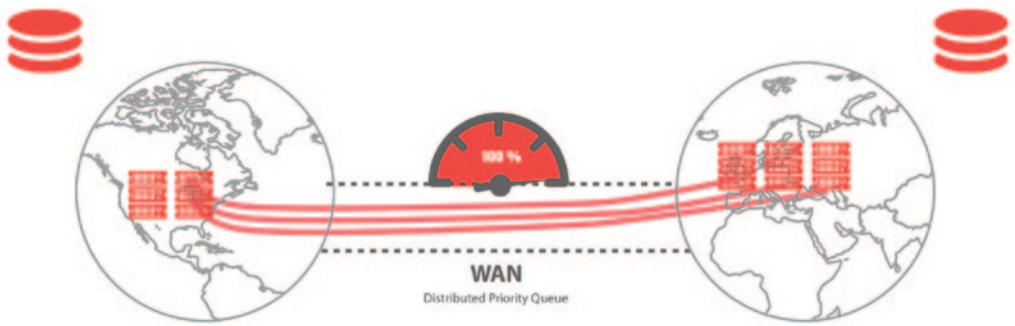
- Simple deployment based on Docker containers using a friendly command line client.
- Easy storage support for user requests based on secure tokens.
- Complex monitoring information available on all aspects of the system, accessible through REST API or directly visualized in the administration panel of the Graphical User Interface.
- Support for multiple storage backends including POSIX based storage (e.g. Lustre), Amazon S3, Ceph, OpenStack SWIFT, and GlusterFS.

Features for developers

- Easy integration with Onedata services using REST API and CDMI protocols.
- Flexible authentication and authorization of requests based on Macaroon tokens.
- Complete reference documentation of the REST API including sample clients for several programming environments.

Onedata users

Onedata has been deployed and evaluated in several initiatives in Europe including Polish National Grid infrastructure PLGrid, INDIGO-DataCloud, EGI DataHub, Human Brain Project and Helix Nebula Science Cloud. In HBP it has proven to meet the users' hard requirements of real-time brain visualization use case.



More information: *https://onedata.org*

Model Execution Environment

The Model Execution Environment (MEE) is a software stack which facilitates the execution of computational workflows on high-performance computing infrastructures, including those available at ACC Cyfronet AGH. The platform's goal is to ensure that computations can be executed straightforwardly by domain scientists, i.e. researchers who do not possess intimate knowledge of the specifics of interaction with computing clusters and other large-scale computing systems.

Pipelines, steps, and models

Within MEE, computational workflows are represented by the so-called pipelines, i.e., collections of computations (each of which is called a step) where the outcome of one computation provides input for another. MEE provides a wide range of facilities enabling users to design steps, arrange them into pipelines, and execute these pipelines on the available computational resources.

Each step is based upon a collection of computational artefacts (executable code) stored in a Git repository. This is referred to as the model. When a step is called for execution, MEE automatically uploads the requested model to the HPC infrastructure and monitors its performance on the input data provided. Users can select a specific version of the given model when launching the pipeline (based on Git versioning mechanisms), thus facilitating traceability and repeatability of computations.

In addition, pipelines can be executed in either automatic or manual mode. An automated pipeline will be executed in its entirety, while a manual pipeline contains a breakpoint at the end of each step, asking the user to manually request the processing of any subsequent steps. This enables users to

download and review interim results and potentially cancel the execution of pipelines which are not expected to yield useful output, thus preserving computational resources.

All MEE features can be accessed via a user-friendly web-based UI. Furthermore, MEE provides programmatic access, which enables integration with higher-level software tools.

Research data management

As MEE schedules and monitors the execution of computational pipelines on HPC resources, care must be taken to manage the associated research data, ensuring that the appropriate input is made available to the underlying models, and that results can be retrieved from the HPC infrastructure. To this end, MEE provides a set of data management interfaces where users of the infrastructure can upload input files and download results. The platform itself manages HPC data storage resources and provides automatic stage-in and stage-out capabilities for research data, along with a set of top-level UI interfaces for its users.

Security

The Model Execution Environment is integrated with PLGrid authentication and authorisation mechanisms. All users of the PLGrid infrastructure can use their login to authenticate themselves with MEE and subsequently schedule and run computations using their PLGrid accounts. Moreover, MEE makes use of PLGrid computational grants assigned to researchers. Pending computations are executed in the context of specific computational grants, which can be predefined within the platform.

Organisations

Externally, MEE provides a set of distinct workspaces dedicated to individual research teams. These are referred to as organisations. Each organisation has a distinct entry point to MEE (i.e., a distinct URL) and can define its own pipelines and pipeline steps, as well as manage its own set of research data. MEE implements compartmentalisation, where each organisation can be managed separately, providing access to a distinct group of users.

Applications

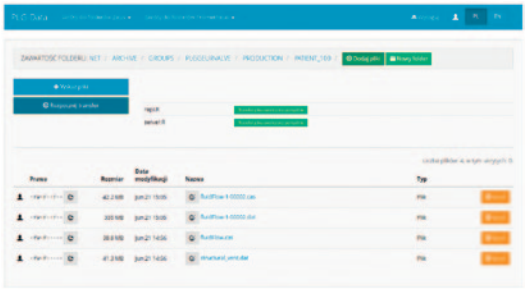
European projects, the POLVAS consortium, and the Sano Centre for Computational Medicine, along with several ad-hoc research collaborations for which individual MEE organisations have been defined. MEE platform was also used as a prototype implementation of the simulation platform for the virtual human twin, developed in the scope of the EU roadmap created by the EDITH project.

https://mee.cyfronet.pl

Simple tool for file management on a computing cluster

PLG-Data

PLG-Data is a tool for the management of data stored in the PLGrid infrastructure. It comes with a user-friendly web interface and allows to upload, download, browse, delete and rename files and folders. It also helps with the management of access rights for members of a research group or external collaborators. It is currently integrated with Ares and Athena supercomputers, and in the future, it may be integrated with new Cyfronet supercomputers.



The set of functionality built into the tool includes, among others, the following:

- downloading files from the cluster to disk,
- adding new files and folders, and removing existing ones,
- renaming files or folders, and changing access rights to them,
- quick navigation to home, scratch and group folders through a handy pull-down menu,
- easy preview of image files without downloading them to a local disk.

Thanks to a specific construction of the URL address to particular files, the tool enables easy sharing of file location with other people, for instance, through copying the browser address bar's content to an e-mail message or an IM communicator. The receiving person will be able to download a file or view the contents of a folder with one click – as long as that person is allowed access to the specific resource.

The service is secured with encrypted HTTPS protocol (between the user's computer and the PLG-Data portal) and the specialised GridFTP protocol (between the service's portal and the computing cluster). The application of such techniques allows the user to manage their files securely. A person who uses PLG-Data does not receive any additional access rights to files stored in the computing cluster, apart from the rights that the person already has.

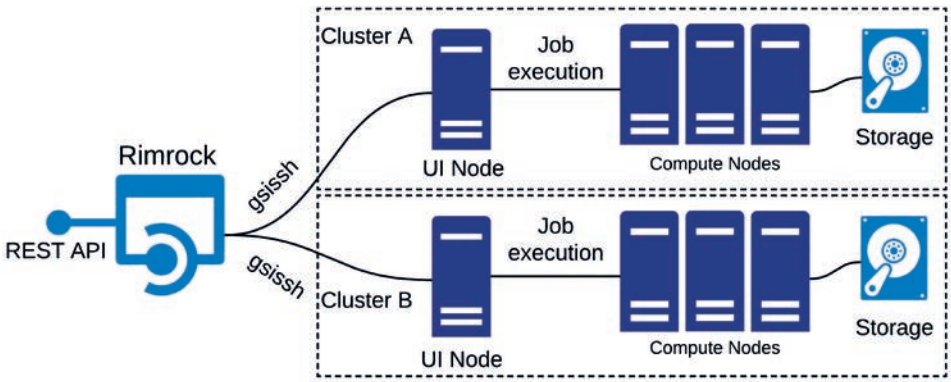
Logging in to the tool is done using the PLGrid user-password pair. The service is available either in Polish or English. An advanced programmer's interface (API) helps developers to integrate their platforms, tools and services with the file storage inside the PLGrid infrastructure.

PLG-Data service address is: *https://data.plgrid.pl*

Rimrock, one of the services of the PLGrid infrastructure, enables the management of scientific computation and result handling with the use of modern interfaces based on REST (Representational State Transfer). REST is a well-established programming pattern often used in applications with distributed architectures. Access to services, applications and advanced scripts deployed on the infrastructure becomes straightforward using REST.

Readiness for various applications

Applying REST principles in implementing the rimrock service allows one to use its functionalities independently of any programming language. It is, therefore, possible to create web and desktop applications as well as prepare advanced computation scripts (e.g. with the use of *Bash* and the *curl* command). An interesting approach also supported by the service is the ability to develop web applications, which can be run solely in the user web browser, minimising the role of server-side software.



Support for several job management systems

The rimrock service uses the Slurm job management system, which ensures support for its unique features. It allows for easy integration of legacy applications in newly developed systems.

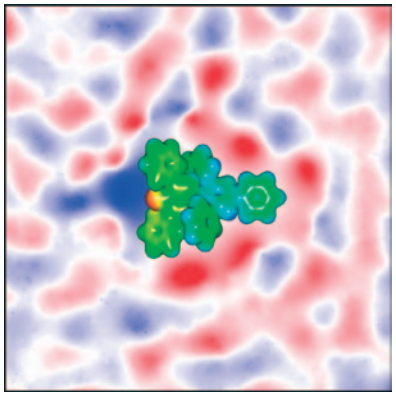
Data security

Data exchanged with the rimrock service is transferred with secure HTTPS connections, and for user authorisation a temporary user certificate (so-called *proxy*) is used.

https://submit.plgrid.pl

Chemistry and Biology – electronic structure and molecular dynamics software

Modern computational chemistry requires constantly increasing resources. More and more computational power is needed to make large systems (especially current challenges of nanotechnology or biological sciences) tractable and improve the accuracy of obtained results. Fortunately, constant progress in computer technology and specialised software offered by Cyfronet meet this demand and enable various chemical computations.



A. Eilmes, P. Kubisiak: Electrostatic potential of an ionic liquid around the solvated dye molecule

Cyfronet clusters' nodes provide up to 1.5 TB of RAM and 48 cores per physical node, which enables quantum chemical computations that require a large amount of memory or a high number of cores with shared memory. Moreover, the fast InfiniBand interface allows good speed-up of calculations if distributed over many nodes. Various quantum chemistry codes also need fast and broad I/O for storage systems. The parallel-distributed Lustre scratch file system and the possibility to use RAMDisk on selected nodes enable that.

Efficient quantum chemistry computations also rely on efficient installation of scientific software and its proper usage. Our administrators' team has the necessary skills, knowledge and experience in installing various applications and efficient running computations. Our portfolio of software used in chemistry contains many packages. Among them, there are:

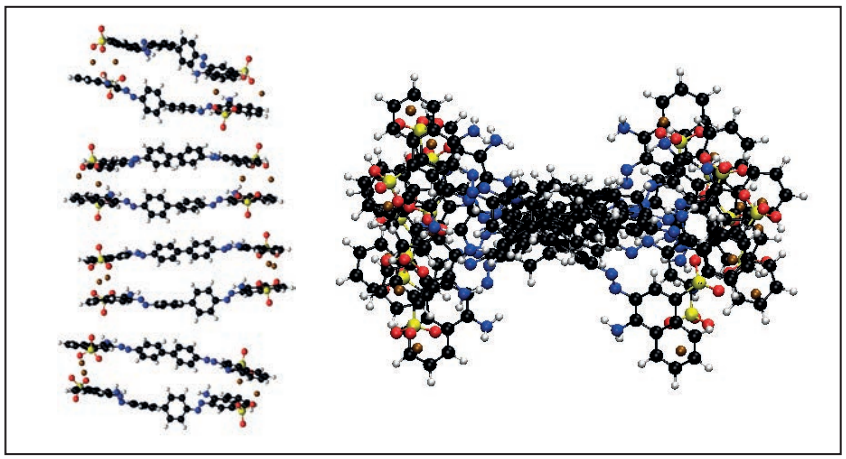
- Versatile and widespread used quantum chemistry codes such as **Gaussian**, **GAMESS US**, **NWChem**, **Schrödinger**, **Q-Chem, Psi4, ORCA** and **TURBOMOLE**, which are capable of calculating electronic structure and various properties of diverse molecular systems using both *ab initio*, density functional theory and semi-empirical methods.

- **Molpro**, **CFOUR** and **Dalton** suites to analyse chemical systems with great accuracy using sophisticated methods such as CC (up to CCSD(T)) and MCSCF.

- Amsterdam Modeling Suite **(AMS, DFTB, MOPAC, COSMO-RS)** provides methods to examine various properties (especially spectroscopic, such as NMR and ESR spectra) of molecular systems with reliable relativistic ZORA approach, COSMO-RS method and all-electron basis sets for the whole periodic table. With addition of versatile and well-constructed GUI of AMS (**AMSInput**, **AMSViev**, etc.) ADF package is used by many of our users.

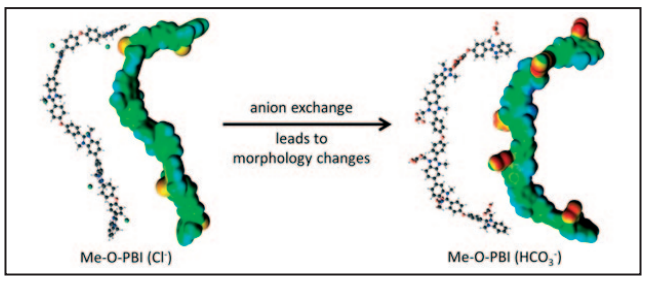
- Several packages, which could be used for solid-state systems. Among them **BAND**, **Quantum ESPRESSO** and **SIESTA** are worth mentioning.

- **AlphaFold** using machine learning to analyze the geometric structures of proteins.
- **Desmond**, **Gromacs**, **Amber**, **LAMMPS**, **NAMD**, **Tinker-HP**, **CPMD**, **CP2K** and **Terachem** suites for molecular mechanics and molecular dynamics simulations of systems containing hundreds of thousands and more atoms.



O. Klimas: Optimized stack of eight Congo Red molecules seen from different perspectives

Nowadays general-purpose computing on graphics processing units (**GPGPU**s) in many scientific domains provides great speed-up of calculations (up to several orders of magnitude). In our computing Centre, some of nodes provide possibility of such calculations on **CUDA** enabled **GPGPU**s (up to eight cards per node). Among software prepared to run on graphical processors our administrators' team prepared quantum chemical packages such as **GAMESS**, **Terachem**, **NAMD**, and **Quantum ESPRESSO, Tinker-HP**. Our experts extensively collaborate with several, mentioned above, packages developer teams. The Cyfronet team prepares and helps with adjusting the dedicated computing environment for our users.



Electrostatic potential of molecules in anion exchange membrane. Published by W. Germer, J. Leppin, C. Kirchner, H. Cho, H. Kim, D. Henkensmeier, K. Lee, M. Brela, A. Michalak and A. Dyck in Macromol. Mater. Eng. 2015, 300, 497–509

Machine learning (ML) and artificial intelligence (AI)

AI-accelerated data analysis is making great strides in many research domains, including materials as well as life science, linguistics and social science. The ability of neural networks to learn from complex data may significantly improve data analysis, classification and pattern detection, with potential applications in many systems, including image recognition, language processing and optimisation.

The Cyfronet supercomputing centre faces up to these challenges and prepares several packages:

PyTorch is a package, specifically a machine learning library for the Python programming language, based on the Torch library. It enables implementation of complex Deep Learning algorithms from the Natural Language Processing, video and images processing and many other areas. It can be used for modeling new architectures in the field of machine learning with focus on experiments.

TensorFlow allows, like Pytorch, to implement models based on the tensor flow paradigm. Due to its character and static representation graph, it allows for efficient optimisation of models training and inferences with respect to the computing platform.

Keras is a library used for designing neural models. It is an external API for engines based on TensorFlow, Microsoft Cognitive Toolkit, Theano, or PlaidML. It has been designed to enable fast experimentation with deep neural networks. It focuses on being user-friendly, modular, and extensible.

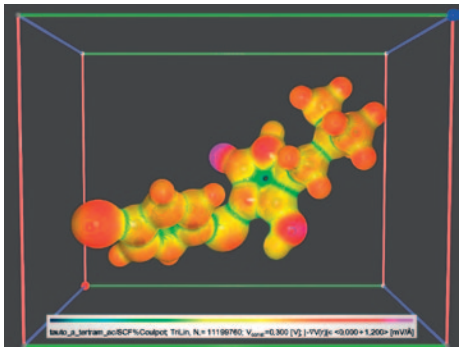
Scikit-learn is a software machine learning library for the Python programming language. It features various classification, regression and clustering algorithms including support vector machines, random forests, gradient boosting, k-means and DBSCAN. It has been designed to interoperate with the Python numerical and scientific libraries NumPy and SciPy.

SchNet is a deep learning architecture that allows for spatially and chemically resolved insights into quantum-mechanical observables of atomistic systems.

Horovod is a distributed training framework for TensorFlow, Keras, PyTorch, and MXNet. The main goal of Horovod is to make distributed Deep Learning fast and easy to use.

Data Visualization, POVRay/ScPovPlot3D

Data visualisation enables analysis and understanding of the results of even very complex numerical calculations, especially multidimensional or time-dependent. Most applications for numerical calculations have a module that generates their visualisation. Python has a matplotlib or VTK+ module, while Matlab or R also have graphic libraries. The situation is similar with regard to geovisualisation programs (GIS) or chemical calculation programs. Unfortunately, no matter how much these programs are refined, the result of their operation is limited by the Cartesian product of available (and compatible) options.

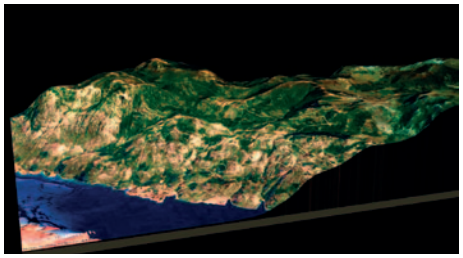


Janusz Opiła: Electrostatic field configuration around the polymer molecule. An equipotential surface with a trilinear approximation is shown, color encodes the electric field intensity module

Overcoming of this limitation, at least for the purpose of creating a prototype of visualisation style for later implementation in a dedicated package, is possible, but requires using a general purpose graphics program, for example 3DMax, Blender or POVRay. However, only the latter is equipped with a scripting language (*Scene Description Language* – SDL), which allows for programmatic, non-interactive creation of visualisations, so is useful for mainframes. As the use of countless SDL language options requires quite persistent studies, a dedicated API was written in the form of a set of specialised modules named the "ScPovPlot3D". This is not a completed project as further extensions are still being added. Thus it may be called a beta version, but mature and working. Currently, the project is in version 4.0 and is hosted on GitHub (URL: *https://github.com/JustJanush/Plot3Dv4*) – the multiplatform API requires POVRay at least in version 3.7.

The most important modules are:

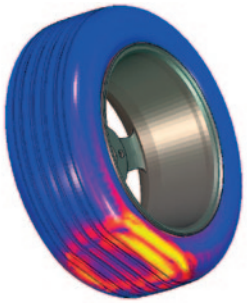
- VectorField.inc – hybrid vector field visualisation using widgets and/or field stream tubes,
- Potential.inc – hybrid visualisation of scalar fields, on regular and irregular meshes with trilinear or centripetal Catmull-Rom cubic interpolation,
- BPatchSurf.inc – hybrid surface visualisation based on data on regular or irregular grids with implemented simple kriging (KDE),
- Mesh2Surf.inc – hybrid visualisation of data defined on regular 2D grids (z=f (x, y)),
- TextExt.inc – extended 3D text formatting, oriented to the presentation of mathematical formulas.



Janusz Opiła: Terrain visualisation based on altitude data collected on an irregular grid and textures obtained from the Google Earth Pro application vicinity of Karlobag, Croatia). Own study: DOI: 10.23919/MIPRO.2018.8400037

If necessary, the package's developer provides technical support. Contact information: *https://skos.agh.edu.pl/osoba/janusz-opila-2390.html*

CAD/CAE applications



Computer-Aided Design and Computer-Aided Engineering applications are essential tools in developing and building almost everything – from car parts to buildings. Through computer simulations, engineers can check the durability of constructs and devices; perform linear and non-linear structural analyses of contact phenomena, plasticity, recoil, etc. CAD/CAE software provides analysis of thermal conductivity, radiation and phase shifts. Significant for science are also fluids simulations: velocity fields, pressure fields, heat distribution, chemical reactions, etc.

Cyfronet's users can resolve all these tasks thanks to CAD/CAE packages of ANSYS, ABAQUS, FLUENT, MARC and OPERA.

ANSYS is a complex structural simulation package with an intuitive graphical user interface, supporting scientists from nearly any area of science or business. Results are calculated with high precision and may be presented by plots or tables, for example, isosurface diagrams and deformations. Computational capabilities of ANSYS are very high and involve: harmonic and spectral analysis, statistics and dynamics.

ABAQUS is devoted to solving problems in the industry using finite-elements analysis. A user can prepare a combination of finite-elements, materials, procedures of analysis and sequences of loads, according to individual requirements, to simulate vehicle loads, dynamic vibrations, multibody systems, impacts, crashes and much more.

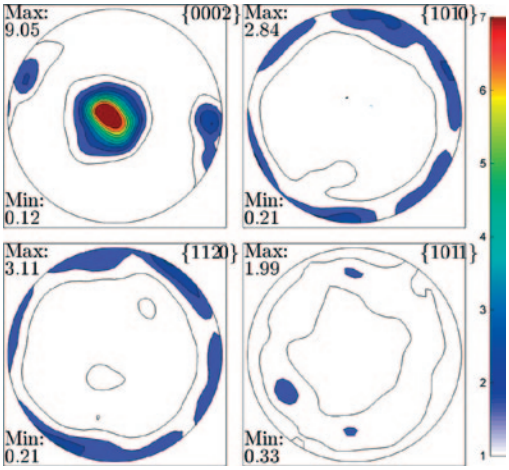
FLUENT software offers the broad physical modeling capabilities needed to model flow, turbulence, heat transfer and reactions for industrial applications ranging from air or liquid flow to semiconductor manufacturing. FLUENT can be used in numerous science domains, including chemistry, metallurgy, biomedicine, electronics, material design and many others.

MARC is a general-purpose, non-linear finite element analysis solution to accurately simulate the product behavior under static, dynamic and multi-physics loading scenarios. It can simulate all kinds of non-linearities, namely geometric, material and boundary condition non-linearity, including contact. It is also the solution that has robust manufacturing simulation and product testing simulation capabilities, with the ability to predict damage, failure and crack propagation. All that can be combined with its multi-physics capabilities that helps couple thermal, electrical, magnetic and structural analyses.

OPERA is a finite element software suite for design and optimisation of electromagnetic devices in 2D/3D. It gives accurate numerical solutions for problems from multiple areas of science, including electrostatics, magnetostatics, low and high frequency electromagnetics. The software gives an ability to design and optimise many types of electrical devices: transformers, motors, switches, micro-machines, MRI scanners and X-ray tubes. It is a powerful virtual prototyping facility to accelerate the design process.

Symbolic math applications

Mathematical applications enable to conduct in reasonable amount of time even very complex and complicated calculations. Users of ACC Cyfronet AGH have access to software that supports calculations in the field of algebra, analysis, combinatorial math, statistics, theory of numbers, geometry or other math areas. Running calculations like integration, differentiation, symbolic processing, matrix operations, approximation and interpolation, Fourier and Laplace Transforms, digital signal processing, etc. is a lot easier. Results can be visualised with appropriate tools. Some of the applications can create interactive 2D and 3D plots. In scientific work, preparation of precise model that most accurately describes analysed issues, is essential.

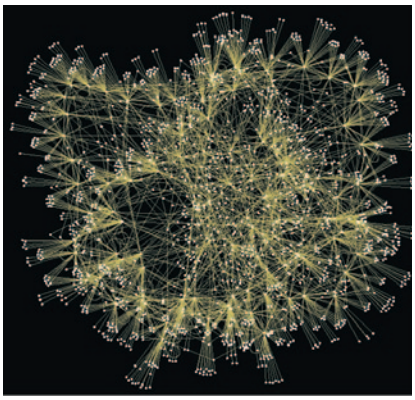


Bartosz Sułkowski: Results of texture simulations by visco-plastic self-consistent model of Zn after hydrostatic extrusion at 250 °C

A good example of software environment, which can be applied in above-mentioned issues, is **MATLAB**. Its modules (Toolboxes) allow performing computations in the field of financial modelling, partial differential equations, linear and non-linear optimisation and much more. It is also possible to use Simulink – the environment oriented for simulations and visualisations from blocks, without the need for traditional programming.

Apart of that environment, users can find in our software a useful application, **MATHEMATICA**, which allows parallel computations with defined precision, dedicated for symbolical and numerical calculations. An advantage of MATHEMATICA is, among other things, a tool for fixing mistakes.

Another example of universal and interactive mathematical software is **MAPLE.** It can be used for simplification of expressions and symbolic processing. It offers databases, enables code generation in other programming languages, creating slideshows with user commands and communication with MATLAB and CAD systems.



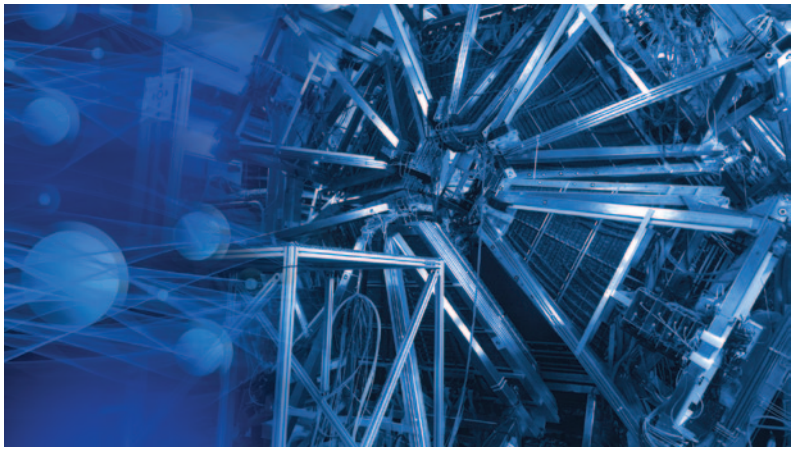
Rafał Rak: One minute price returns network for KGHM (the Polish stock company)

Dynamically developing scientific research requires more and more advanced tools nowadays. Among them, IT tools play a huge role, supporting the effective research from the moment of its design to the development of results.

Cyfronet, by following the latest solutions and creating its own studies, tries to fulfill an important area of its mission to support science.

Dedicated laboratories were established for these needs.

Laboratory of Quantum Computing



The Laboratory was established to conduct research on the use of quantum computers in calculations and to support classical calculations with quantum accelerators.

One of the key tasks is to follow the development of quantum computing technologies and available quantum accelerator platforms in order to use them in dedicated services offered by Cyfronet. We cooperate with other research entities and industrial partners, both as consortium members of joint initiatives and carrying out commissioned works.

Based on our own competences and the exchange of expert knowledge with a network of partners, our team is working on solving the problems that prevent us from wider and more effective using the quantum accelerators in calculations for the benefit of science and economy.

We also act to popularize calculations using quantum accelerators and provide substantive user support. In this regard, we prepare the necessary documentation and materials, conduct training and publish the results of research work.

Contact: Mariusz Sterzel, m.sterzel [at] cyfronet.pl

Laboratory of Information Methods in Medicine

The main tasks of the Laboratory focus on two spheres. The first is research activity, which includes a thorough analysis and verification of available and potential answers to the challenges found at the border of medicine and information technology. The second one covers the design, development and subsequent operation of dedicated applications and platforms for medical applications. This scope also

covers the monitoring of the security status of the developed software as well as data storage and processing mechanisms.

Thanks to the comprehensive approach to the processes: from the identification of the research problem, through the analysis of users' needs, to the final implementation, the Laboratory effectively implements its mission to support the scientific and medical community. As part of the dissemination of expert knowledge, members of the Team publish research results in scientific journals, participate in the preparation of information materials and conduct consultations for users.

Laboratory employees establish cooperation with renowned domestic and foreign research institutes and medical IT centers. The effects of this cooperation are, among others, ongoing and already implemented projects with significant participation of Team members:

- Sano: Centre for New Methods in Computational Diagnostics and Personalised Therapy,
- PRIMAGE: PRedictive In-silico Multiscale Analytics to support cancer personalized diaGnosis and prognosis, Empowered by imaging biomarkers,
- Virolab: A Virtual Laboratory for Decision Support in Viral Disease Treatment,
- Gliomed: Diagnostics of gliomas based on the slowly circulating DNA of the tumor,
- Eurvalve: Personalised Decision Support for Heart Valve Disease,
- CECM: A Centre for New Methods in Computational Diagnostics and Personalised Therapy.

The previous activity of the current Laboratory team is presented in detail on the following website: *http://dice.cyfronet.pl*.

Contact: Marian Bubak, bubak [at] agh.edu.pl

Laboratory of Data Processing

The Laboratory designs and implements dedicated applications and software platforms for applications in various fields of science. The Laboratory consists of specialists in the field of software architectures, Front-end and Back-end programming, user interface and user experience design, DevOps, testing, and requirements analytics. The team specializes mainly in:

- development of innovative methods of acquiring knowledge from available data,
- development of technologies supporting open data processing,
- integration of data and knowledge processing systems with existing repositories and e-infrastructures.

The Laboratory establishes cooperation with renowned scientific and research units as part of Polish and international projects. The effects of cooperation include:

- **Construction of the Sat4Envi Portal** (*https://dane.sat4envi.imgw.pl*), providing satellite data from the Copernicus program. The portal enables searching, viewing, ordering and downloading satellite data and their derivative products using only a web browser.
- **Development and maintenance of the EOSC Portal** (*https://eosc-portal.eu/*) as part of a series of projects related to the European Open Science Cloud (EOSC). The portal provides access to the resources of many European e-infrastructures and research infrastructures through a unified user authentication system. EOSC activities focus on the implementation of the Open Science paradigm.

In 2022, the new Laboratory of Interdisciplinary Scientific Computing was separated from the Laboratory of Data Processing.

Contact: Roksana Wilk, r.wilk [at] cyfronet.pl

Laboratory of Interdisciplinary Scientific Computing

The Laboratory conducts research and development work on the processes of conducting and supporting scientific calculations and the organization of scientific data. The Science Gateways portals elaborated by the Laboratory employees create the possibility of establishing cooperation with external entities: Polish and foreign.

The Laboratory tasks are also focused on:

- implementation of research grants and industrial orders,
- using expert knowledge to solve problems requiring the use of various computing resources, e.g. machine learning technology,
- popularisation of calculations using the tools created by the Laboratory among users,
- essential support for users, realized among others by monitoring needs, developing documentation, and conducting training.

The team of the Laboratory, previously co-creating the Laboratory of Data Processing, developed the proprietary InSilicoLab programming environment, which includes a set of advanced tools and programming libraries that allow for the construction and development of dedicated research portals. Portals based on InSilicoLab are designed in such a way as to gather in one place all the tools that researchers need for *in silico* calculations.

The main advantages are:

- easy running of the user experiments, even if they are complex, long and require many calculations,
- the ability to conveniently describe, categorise and search for input or output data.

The InSilicoLab technology is distinguished by striving for the greatest possible usability of the tools built with the help of the environment. This sphere includes both the usefulness for solving scientific problems in a given field, as well as the user-friendliness of the portal for its end-user.

The effects of the Laboratory team cooperation with renowned scientific and research units as part of Polish and international projects include the development of the **EPISODES Platform** (*https://tcs.ah-epos.eu/*) as part of a series of projects related to the European Plate Observing System - EPOS (*https://www.epos-eu.org/*).

The portal and the tools organized around it are focused on the study and analysis of seismicity and other phenomena caused by human activity (e.g. exploitation of resources within a mine, creation of artificial water reservoirs). The portal is integrated with the European EPOS infrastructure.

Contact: Joanna Kocot, j.kocot [at] cyfronet.pl

Laboratory of Cloud Technologies

The Laboratory deals with the design and operation of the cloud for science, as well as tools for its effective use. The team is developing comprehensive environments for access to distributed data, taking into account both the issues of secure data storage and processing in the cloud, as well as convenient access interfaces (portals, applications) for the end user.

Bearing in mind the dynamic development of new technologies for processing and storing data in the cloud, the Laboratory constantly conducts research and publishes the results. Using the team's expert knowledge, it actively supports scientific initiatives, including international projects and e-infrastructures.

The flagship product of the Laboratory is **Onedata**: a globally scalable data management system, unifying access to data stored in distributed systems. Onedata responds equally well to the needs of both small user groups and large international research communities. The system enables users to use a homogeneous data management system for both personal and work-related data storage, such as research results, and enables accessing it efficiently from any device.

More information at: *https://onedata.org*.

Contact: Łukasz Dutka, l.dutka [at] cyfronet.pl

ACC Cyfronet AGH at the IGF Poland 2023 Digital Summit in Wroclaw

On October 4, 2023, representatives of Cyfronet AGH took part in the Internet Governance Forum Poland, where they gave the presentation titled „Supercomputers not only for science – opportunities and access". The presentation and the following discussion covered the applications of supercomputers and related technologies – artificial intelligence, large-scale data processing, and quantum computers – for developing science, improving public administration's functioning, and supporting industry development.

The offer of the National HPC Competence Center (EuroCC Poland) and the PLGrid infrastructure was also presented regarding access to Polish supercomputing resources, training, and user support.

The National HPC Competence Center is an expert center coordinated by ACC Cyfronet AGH and a contact point that helps use the Polish and European supercomputing infrastructure.

The EuroHPC PL project team was the winner of the Polish Smart Development Award 2023

On October 20, 2023, during the Intelligent Development Forum 2023 in Uniejów, the Polish Smart Development Award winners were announced. In the "Project of the Future" category, the award was given to the „National Supercomputing Infrastructure for EuroHPC - EuroHPC PL" project, coordinated by Cyfronet AGH. The award was granted „for the results of projects that may positively impact socio-economic development, as well as an open approach to promotion and communication with the public to present the importance of the benefits resulting from the implemented solution".

On behalf of the project, the award was received by Marek Magryś, Deputy Director of ACC Cyfronet AGH for High-Performance Computers at that time and coordinator of the EuroHPC PL infrastructure. Henryk Baniowski, Deputy Director of ACC Cyfronet AGH for Cybersecurity and Innovative Economy, also participated in the event.

The awards gala ended the two-day Smart Development Forum, during which representatives of ACC Cyfronet AGH promoted the achievements of the EuroHPC PL project and the possibilities of using them by representatives of science and innovative economy.

During the event, at the „Digital Transformation and Intelligent Automation using Analytics and Artificial Intelligence" conference, Marek Magryś gave a presentation entitled: „National Supercomputing Infrastructure for EuroHPC - EuroHPC PL" and participated in a panel discussion.

– *The Smart Development Award shows that the development of Polish computing infrastructure is crucial for the further development and support of innovation of the entire country* – said Marek Magryś after the event. – *I would like to thank everyone who implements and supports activities for the National Supercomputing Infrastructure for EuroHPC – EuroHPC PL, particularly Cyfronet and project partners' teams.*

Cyfronet Open Day 2023

Every year, the Academic Computer Center Cyfronet AGH organises an Open Day for the scientific community of Krakow and the Małopolska region.

The program of the event includes:

- presentation of Cyfronet's activities and information about hardware resources, software and ongoing projects,
- presentation of the latest trends in the development of computer and network architectures, including resources that allow performing quantum calculations,
- speeches on the computational capabilities of supercomputers and their application for the analysis of research results, simulations, visualization, and parallel analysis of huge data sets (big data), including for the development of artificial intelligence,
- announcement of the results of the competition for the best doctoral thesis based on the Cyfronet computing resources and presentations of the winners.

Participants of the Open Day have the opportunity to get acquainted directly with the unique services of Cyfronet and the possibility of using them in research for the synergy of science and economy.

The EuroHPC PL project conference

On December 7-8, 2023, at the Auditorium Maximum of the Jagiellonian University in Krakow, a conference was organized summarizing the project „National Supercomputing Infrastructure for EuroHPC - EuroHPC PL", implemented in 2021-2023. The two-day conference program included the presentation of:

- achievements made within each task and the overall achievements of the project,
- hardware resources (supercomputers and accelerators) and intangible resources (procedures, software) created in the project,
- quantum resources made available thanks to the project,
- the LUMI and LUMI-Q infrastructure and their integration with the EuroHPC PL infrastructure.

One hundred thirty participants attended the conference.


Narodowa Infrastruktura Superkomputerowa
dla EuroHPC - EuroHPC PL
TECHNOLOGIE INFORMATYCZNE
PRZYSZŁOŚCI


Narodowa Infrastruktura Superkomputerowa
dla EuroHPC - EuroHPC PL

HPC Users' Conference (KU KDM) 2024

The basic premise of the HPC Users' Conference was to initiate annual scientific meetings devoted to users performing computations in ACC Cyfronet AGH with the use of high-performance computers, computing clusters and installed software.

The conference was launched in 2008 and included several presentations by Cyfronet employees – describing the resources available in the Centre, as well as numerous lectures of researchers – presenting the scientific results achieved using Cyfronet hardware and software. In addition, two invited speeches were given – by Norbert Attig from Jülich Supercomputing Centre and Jaap A. Kaandorp from the University of Amsterdam.

The first edition of the conference attracted much attention and increased the interest of users in Cyfronet resources. It proved that this type of event was much awaited and needed.

Nowadays, the HPC Users' Conference focuses on large -scale computations and simulations, novel algorithms in computer science, tools and techniques relevant to high-performance computing, teaching in computer science, databases. However, the main aim of the conference is the overview of research results carried out using the computer resources of Cyfronet. It is also an opportunity to familiarize the users with the Centre and its resources, including the PLGrid infrastructure.

The conference includes a series of talks by scientists who perform research using Cyfronet resources and can present the role of these resources, typical usage scenarios and performance aspects. The event is an important opportunity for Cyfronet representatives to meet with these scientists and acquire the knowledge necessary to take the proper actions in order to adapt the computing infrastructure to scientists' needs and fulfil their requirements. On the other hand, the conference also gives a possibility for researchers representing various disciplines to exchange experience and become familiar with the new technologies and services currently being deployed at the Centre.

The crucial parts of the conference are meetings with suppliers of Cyfronet hardware and software, as well as the panel discussion on the efficient use of these resources. The latter is always attended by users – researchers, who use the chance to get familiar with news regarding the computing infrastructure in the Centre and to inform Cyfronet experts about issues encountered while interacting with this infrastructure.

Contributed papers elaborated on the basis of the best conference talks are published in one of two well-regarded IT journals: Computing and Informatics (CAI) (*http://www.cai.sk*) or Computer Science (CSCI) (*www.csci.agh.edu.pl*).

https://www.cyfronet.pl/kukdm24

The Polish Open Science 2024 Conference

The Polish Open Science 2024 Conference was organized in Krakow on April 10-12, 2024. The Conference is a unique event in Poland, devoted to issues related to various aspects of Open Science, bringing together all stakeholders related to the collection, sharing, and management of research data, creation of repositories and scientific infrastructures, development of initiatives related to EOSC, sharing publications, articles, and monographs in Open Access, as well as issues related to openness in the context of scientific evaluation.

It is an event created by and for the Open Science community and the only one that invites researchers, scientific communities, librarians, data stewards, creators of scientific infrastructure, tool suppliers, IT specialists, publishers, and various organizations to discuss and exchange experiences. In the formula of scientific and professional discussion, the conference is a platform shaping the Open Science environment in Poland, showing experiences, trends, and challenges facing Open Science initiatives worldwide, in the region, and Poland.

The conference draws on the tradition of the Pomeranian Open Science Conference, six editions of which were held in 2017-2022.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LUMI Day Poland 2024 conference

On February 29, 2024, an online conference was organized to present the LUMI supercomputer, the path of applying for its resources, and the possibilities of its use by Polish scientists.

The LUMI supercomputer, built by a consortium covering ten countries, including Poland, has been ranked 8th on the TOP500 list of supercomputers with the highest computing power in the world.

Details about LUMI can be found at *https://cyfronet.pl/lumi*.

Polish scientists can access LUMI via the national PLGrid infrastructure (*https://portal.plgrid.pl/*).

Topics covered at the conference included:

- LUMI's place in the European EuroHPC JU initiative,
- scientific challenges to be answered thanks to LUMI,
- application path for LUMI supercomputer resources,
- support for LUMI supercomputer users,
- software in a pre-exascale environment,
- examples of using LUMI supercomputer resources,
- EuroCC – National Competence Centers in the framework of EuroHPC
- the Epicure project.

LUMI supercomputer, photo: Fade Creative

ACC Cyfronet AGH at the ISC High Performance 2024 in Hamburg

ISC High Performance (The Event for High Performance Computing, Machine Learning, Data Analytics & Quantum Computing) is one of the most important events for the community of providers and users of solutions related to large-scale computing. The event was held on 12-16.05.2024 and traditionally consisted of a conference covering virtually all areas related to the application of supercomputing, as well as an industry fair, allowing direct presentations of equipment, projects, and solutions.

Representatives of Cyfronet participated in the conference, learning about the latest technologies and examples of their applications. During the conference, Marek Magryś, Cyfronet's Deputy Director for HPC at that time, received a certificate for the Helios supercomputer's 3rd place on the prestigious Green500 list of the world's most energy-efficient supercomputers. In addition, the TOP500 list of the world's fastest supercomputers was also announced, on which Cyfronet's machines took four places.

Cyfronet appeared at ISC as an exhibitor for the fourth time, this time under the slogan "Access the future." Cyfronet's participation at ISC was, among other things, related to promotional activities under the "EuroHPC National Competence Centers, Phase 2" project. The information and promotional stand of ACC Cyfronet AGH was one of the few Polish accents during the fair. Among the exhibitors were both companies – technology giants such as Hewlett Packard Enterprise, Intel, and NVIDIA, as well as leading supercomputing initiatives and centers, including EuroHPC JU, LUMI, and Jülich Supercomputing Center. In total, 160 exhibitors from 30 countries participated in the fair.

The main activities of Cyfronet during the ISC included:

- maintaining and developing relationships with existing partners,
- establishing new contacts with potential hardware and software suppliers,
- evaluating new technological solutions that can be implemented within the managed infrastructure.

This year's ISC High Performance attracted some 3,400 participants from all around the world.

Cyfronet is the leader of projects included on the Polish Research Infrastructure Map

Among the strategic infrastructures included in January 2020 on the Polish Research Infrastructure Map there are two projects proposed by ACC Cyfronet AGH as the initiator and coordinator of the PLGrid consortium: *National Supercomputing Infrastructure for EuroHPC* and *National Cloud Infrastructure PLGrid for EOSC*.*

The aim of the **National Supercomputing Infrastructure for EuroHPC** program is to build a computing infrastructure for scientific research on solutions that meet the current and future needs of Polish society, the scientific community and the economy.

The infrastructure will be based on modern supercomputing systems enabling the implementation of both traditional simulation tasks and data analysis using artificial intelligence methods. The production computing systems built within the project will be among the world's leading supercomputers. In addition to the computing infrastructure, the project will also provide access to specialized training and expert technical support for users from science and economy, as well as the necessary procedures concerning allocation and accounting of used resources.

As a result of the implementation of the National Supercomputing Infrastructure for EuroHPC project, an infrastructure for conducting research for the needs of science, economy and society will be created, benefiting from the latest HPC technologies developed within the international EuroHPC cooperation. The infrastructure will offer services in the fields of massively parallel computer simulations, highly efficient processing of data sets, the use of artificial intelligence methods, software and high productivity tools, including data visualization, and user support and training.

Within the National Supercomputing Infrastructure for EuroHPC programme the EuroHPC PL project was accomplished, with the Helios supercomputer as its greatest achievement.

National Cloud Infrastructure PLGrid for EOSC is a program for the use of cloud resources for scientific research that meets the current and future needs of the Polish society, the scientific community and the economy. The scope of this research includes data, infrastructures and data processing platforms, as well as effective algorithms and dedicated applications.

The program is based on the requirements of the society, economy and Polish researchers, in particular those cooperating within international research groups. These groups require advanced environments for the integration of distributed resources: software, infrastructures and dedicated services. These requirements can only be met by advanced IT technologies combined with computing, storage and data resources. Cloud technologies enable the interaction of all these elements within a flexible ecosystem.

National Cloud Infrastructure PLGrid for EOSC is part of the ecosystem of the European Open Science Cloud (EOSC, Declaration of 26.10.2017). Poland is currently developing two key components of this federated, globally available and multidisciplinary environment: Onedata – a system for unified data sharing and management, and the EOSC Portal. As part of the European ecosystem, the PLGrid National Cloud Infrastructure will offer trusted and open environments for users throughout the data lifecycle. This will allow scientists, the economy and society as a whole to publish, search, use and re-use the collected data, tools, software and other results.

The research planned within the National Cloud Infrastructure PLGrid for EOSC will allow for the development, validation and, consequently, the provision of services (general and dedicated), and thus the use of modern technologies and effective techniques for management, processing and reusing data by scientific communities, economic entities and society.

Within the National Cloud Infrastructure PLGrid for EOSC the PLGrid ICON project has been launched.

**Material from the "Polish Research Infrastructure Map" brochure of the Ministry of Science and Higher Education.*

Bielik - the first Polish language model

Bielik-11B-v2 was created as a result of the work of a team working within the SpeakLeash Foundation and the Academic Computer Centre Cyfronet AGH and is a Polish model from the LLM (Large Language Model) category with 11 billion parameters. The team's work on the Polish language model lasted more than a year, and its original scope included data collection, processing, and classification. Currently, the SpeakLeash Foundation's resources are the largest, best-described, and most documented collection of Polish language data.

Helios and Athena – computing power for science

Supercomputers from ACC Cyfronet AGH allowed the Bielik project to spread its wings. The support of our team also concerned the optimization and scaling of training processes, work on data processing pipelines and the development and operation of synthetic data generation methods, as well as work on model testing methods. Valuable experience and knowledge gained from this cooperation enabled PLGrid's team of experts to prepare guidelines and optimized solutions, including computing environments for working with language models on the basis of Athena and Helios supercomputers for the needs of scientific users.

– *We used the resources of Helios, currently the fastest machine in Poland, to teach language models* – specifies Marek Magryś, Acting Director of ACC Cyfronet AGH. – *Our role is to support the process of cataloging, collecting, and processing data with expertise, experience and, above all, computing power, and to carry out the process of teaching language models together. Thanks to the work of the SpeakLeash team and AGH, we were able to create Bielik, an LLM model that perfectly handles our language and cultural context, and which can be a key component of text data processing chains for our language in scientific and business applications*.

The computing power of Helios and Athena in traditional computer simulations is a combined total of more than 44 PFlops, and for lower-precision artificial intelligence calculations, it is as much as 2 EFlops.

If we are operating with such large data as in the case of the Bielik project, then, of course, the infrastructure needed for the work exceeds the capacity of an ordinary computer. We must have the necessary computing power to prepare the data, compare it with each other, and train the models. The barrier to the availability of such supercomputers means that only some companies are able to carry out such work on their own. Fortunately, AGH has such facilities – explains Professor Kazimierz Wiatr.

Why is it essential to create Polish language models?

One of the benefits of launching Bielik is strengthening Poland's position in the area of AI innovation. Moreover, as the creators emphasize, it is worth striving to build our own tools and thus become independent of external companies, which, in case of market turmoil, regulations, or legal restrictions may, for example, prevent access to their resources. Thus, by developing and improving tools in Poland, we can build a stable base and secure many of our sectors – banking, administrative, medical, and legal.

The version that users can test is maintained free of charge in the public domain and continues to be improved. The authors have made available, in addition to full versions of the developed models, a range of quantized versions in the most popular formats available, which allow users to run the model on their own computer.

Useful links:

- The possibility to test Bielik: *bielik.ai*
- Actual quantity of collected data: *speakleash.org/dashboard*

EPOS – multidisciplinary platform supporting Earth sciences research

We need to use various tools and research methodologies to monitor the processes ongoing below the Earth's surface effectively and their effects perceptibly on the surface. In this regard, the EPOS – European Plate Observing System aims to deliver complex solutions that cross the borders of different countries and research disciplines.

In October 2018, EPOS was granted the status of ERIC: European Research Infrastructure Consortium. This way, a legal and administrative framework was established, which allows EPOS to carry out international activities not only as a project implemented by many partners but rather as a separate entity with its headquarters in Rome.

The idea standing behind EPOS is to recognise better Earth functioning as a complex system in which, on the one hand, natural episodes (such as volcanic eruptions, floods or earthquakes) have an impact on society and the economy. On the other hand, the environment is being changed by anthropogenic factors. For this reason, effective research requires a multifaceted approach. By integrating European research infrastructures into the transnational system, which delivers data, data products, software and services, EPOS works on enabling access to so far dispersed possibilities. The initiative focuses on ten main, linked with each other, Thematic Core Services (TCS): Seismology, Near-Fault Observatories, GNSS Data and Products, Volcano Observations, Satellite Data, Geomagnetic Observations, Anthropogenic Hazards, Multi-Scale Laboratories, Geo-Energy Test Beds for Low Carbon Energy, Tsunami.

Image: EPOS - European Plate Observing System

Computational Earth sciences

Providing the research infrastructure as an internet platform requires close cooperation of IT specialists with representatives of Earth sciences. Synergic activities are carried out on many levels – starting from measurements and experiments conducted by scientists generating a large amount of raw data, which is stored and processed in information systems – i.a., within Cyfronet's infrastructure. Cooperation is also significantly influential in building data visualisation tools, which are managed from the web browser level using Graphical User Interfaces (GUI). In the long run, EPOS aims to connect research communities within one multidisciplinary platform, provide effective and safe access tools, and develop new services based on previous achievements.

It's worth underlining that geophysical and geological data, advanced visualisation and analytic software will be available in open access and free of charge. Thanks to that, EPOS supports interdisciplinary research on the causes and effects of processes ongoing below and on the Earth's surface.

This is especially important in the light of monitoring environmental threats, such as earthquakes, floods, landslides or volcanic eruptions, and anthropogenic threats related to, among other things, the activities of mines. Through a comprehensive analysis of already observed phenomena, one can better prepare for events that have not yet taken place, limiting their adverse effects as much as possible.

EPOS has entered the operational phase of the infrastructure built within EPOS PP, EPOS-IP, and EPOS SP projects. The EPOS research platform is available at *https://ics-c.epos-eu.org/*, and the portal gathering information about EPOS activities is available at *https://epos-eu.org/*.

Cyfronet's activities for EPOS

ACC Cyfronet AGH is participating in successive projects building EPOS, supporting the initiative with both hardware resources and the knowledge and skills of specialists. Parallel activities include several spheres, one of which is the development of the EPISODES digital platform for one of the EPOS thematic nodes – the Thematic Core Service Anthropogenic Hazards (TCS AH) node.

The platform is available at *https://EpisodesPlatform.eu* and provides a tool for analysing anthropogenic seismicity and associated hazards and for assessing the potential environmental impact of geo-resource exploitation. With data from seismic stations and shared industry information, the platform makes it easier to analyse processes such as the flooding of artificial reservoirs and extraction of raw materials, shale gas or groundwater. In addition to sharing and visualising data, the EPISODES Platform provides a virtual workspace for running applications from different vendors and organising data. It also makes it possible to create your own applications and use them on the aforementioned data, as well as to combine applications into larger experiments – creating a so-called workflow. The functionality was created thanks to the national project – EPOS-PL, while within the framework of another project – EPOS-PL+, the EPISODES Platform was enriched with the possibility of conducting experiments using artificial intelligence.

In addition to creating and maintaining the EPISODES Platform, as well as providing the infrastructure for calculations involving it, Cyfronet specialists take care of maintaining the integration elements between the TCS AH thematic node and the central EPOS Data Portal, which allows access to the results of activities at all EPOS thematic nodes.

In the framework of subsequent European projects, the EPISODES Platform is also being developed in terms of increasing the amount of data available on the platform, adapting the platform's capabilities for industrial research, and integrating the platform's services with those of the European Open Science Cloud (EOSC) – the Geo-INQUIRE (Geosphere INfrastructures for QUestions into Integrated REsearch) and EPOS ON (EPOS Optimization and EvolutioN) projects. The platform is also being developed to adapt to study extreme geophysical conditions within the framework of the "digital twin" being built within the DT-GEO project.

Sano: Centre for Computational Personalised Medicine - International Research Foundation

Owing to a unique initiative carried out in 2019-2026 by the Academic Computing Centre Cyfronet AGH along with five partner institutions in the framework of the EU Horizon 2020 *Teaming for Excellence* programme, the International Research Agendas programme implemented by the Foundation for Polish Science, and with financial support from the Ministry of Science and Higher Education, a new entity called **Sano –** Centre for Computational Personalised Medicine was established in Kraków.

The mission of Sano involves:

- development of new computational methods, algorithms, models and technologies for personalized medicine,
- introducing new diagnostic and therapeutic solutions based on computerized simulations into clinical practice,
- fostering the creation and growth of enterprises which develop cutting-edge diagnostic and therapeutic technologies,
- contributing to novel training and education curricula which meet the needs of modern personalised medicine.

The **Sano Centre** (*https://sano.science/*) is situated in Kraków: a city well known for educating top-class medical practitioners and IT experts, whose teaching hospitals are well regarded among the academic community and whose life science technology sector is continually expanding.

The establishment of the **Sano Centre** directly contributes to regional scientific excellence by fostering new research collaborations and creating top-tier educational opportunities for postgraduate students. It will also improve knowledge and technology transfer by promoting the creation of new commercial enterprises which deal with advanced technologies. The Centre's impact will transcend regional boundaries, contributing to advancements in medical research and thereby to the quality of medical care.

The Centre's objectives are based, among others, on the National Smart Specialisation Strategy. **Sano** aims to enhance collaboration between academic and commercial institutions on an international scale. Key performance indicators include the number of highly cited scientific publications and grants obtained by the Centre, the number of solutions based on computational models which have been introduced into clinical practice, and the number of innovative, marketable products and services.

The Centre for Computational Personalised Medicine represents a joint international collaboration of the following institutions: ACC Cyfronet AGH, LifeScience Cluster Krakow – a Key National Cluster, University of Sheffield and Insigneo Institute, Forschungszentrum Jülich, Fraunhofer Institute for Systems and Innovation Research ISI, and National Center for Research and Development.

Digital Twins

The concept of Digital Twins (DT) assumes the creation of a virtual model that reflects the features of the object adopted as a model as faithfully as possible. This makes it possible to conduct computer analyses to take effective, model-tested actions in reality. Through its infrastructure and expertise, Cyfronet supports the creation of the "Digital Twin" model in various fields of science.

The EDITH project (An Ecosystem for DIgital Twins in Healthcare) developed an integrated system architecture to implement the human "Digital Twin" concept and a vision for its further development. The Cyfronet team coordinated the development of a demonstration prototype of the simulation platform.

In turn, the DT-GEO project (A Digital Twin for GEOphysical extremes) assumes the implementation of a "Digital Twin" prototype to study extreme geophysical conditions, such as earthquakes (natural or anthropogenic), landslides, volcanic eruptions and tsunamis. In this case, Cyfronet specialists are working on the part related to anthropogenic threats.

The InterTwin project (An interdisciplinary Digital Twin Engine for Science) co-designs and implements a prototype of an interdisciplinary solution called Digital Twin Engine (DTE). This open-source platform provides generic and customized modeling and simulation software components to integrate Digital Twins (DTs) specific to the application. In the project, the Cyfronet team introduces integration with the proprietary OneData platform.

The GEMINI project (A Generation of Multi-scale Digital Twins of Ischaemic and Haemorrhagic Stroke Patients) aims to provide validated multi-organ and multi-scale computational models to support therapeutic decisions and improve fundamental understanding of ischemic and hemorrhagic acute strokes. Virtual twin models will be created, which will then be tested on a large scale by the Cyfronet team the same model will be used for a large group of patients using the HPC infrastructure.

The cloud environment

The ability to run a complete work environment in the cloud, with access to distributed hardware resources and software packages, facilitates research in international teams. Cyfronet has been developing cloud "ecosystems" for years based on available open-source tools and proprietary technologies.

The main goal of the INDIGO-DataCloud project (INtegrating Distributed data Infrastructures for Global ExplOitation) was to develop a PaaS (Platform as a Service) environment enabling large-scale computing by integrating grid and cloud resources and providing uniform access to both computing resources and data storage resources. The role of ACC Cyfronet AGH was mainly to implement a consistent system of access to geographically dispersed data stored in heterogeneous repositories.

Based on the project's achievements mentioned above, another project was carried out: XDC (eXtreme DataCloud), which aimed to build specialised solutions for large-scale data management and processing in a hybrid cloud, thus introducing the issues of data access and migration in distributed cloud environments. Cyfronet was responsible for implementing a distributed data management system in a cloud environment.

One of the currently implemented projects is DOME (A Distributed Open Marketplace for Europe Cloud and Edge Services). Based on the assumptions of the Gaia-X program and open standards, tools and procedures are being developed to support the development and adoption of trusted Cloud and Edge services in Europe. The DOME project will be an access point for broadly understood software and data processing services developed under EU programs such as Digital Europe, Horizon 2020, or Horizon Europe.

EOSC – transnational integration of scientific resources

The European Open Science Cloud (EOSC) is an initiative aiming to create a virtual environment that would complete the assumptions of the Open Science paradigm. EOSC aims to share (easily and transparently) research data and advanced tools and resources to store, share, process, and manage this data.

Within EOSC, the connections between currently existing research e-infrastructures are made, and the integration takes place, i.a., by the unification of access and authorisation rules for researchers from different countries. Thanks to the achievements of EOSC-Hub, belonging to the family of EU-funded EOSC-building projects, a platform was created to do this. The EOSC-Portal is the interface between providers of scientific services and resources, and researchers who can benefit from those. ACC Cyfronet AGH team played a crucial role in this regard, becoming the Portal host and developing the Marketplace website, an extensive catalogue of services and documentation provided by EOSC partners.

Further development of EOSC

Development of the Portal and integration of services from the larger group of deliverers are the core assumptions of the planned enhancement of EOSC.

The EOSC Enhance project (*https://www.eosc-portal.eu/enhance*), which was realised from 2019 to 2021, aimed to improve the Portal in terms of convenience and speed of use. The works carried out by our specialists concerned, among others, advanced analysis of user behaviour in order to create and implement the best user experience practices. At the same time, new functionalities have been implemented.

The EOSC Synergy project (*https://www.eosc-synergy.eu/*), which lasted until the end of October 2022, has been underway to implement EOSC standards for another nine national e-infrastructures. Cyfronet, in addition to coordinating activities at the national level, supported the planning process by looking for new, effective solutions for integration in other countries.

The EOSC Future project (*https://eoscfuture.eu/*), which finished in 2024, improved the quality of the EOSC ecosystem so that it supported European research even better and convinced researchers to use the offered resources. This was achieved through further work on the Portal and the integration of new scientific infrastructures and initiatives. Cyfronet's responsibility as part of EOSC Future was the further development of one of the three main pillars of the Portal, which is the part aimed at the users, in particular related to the components supporting the Marketplace.

Cyfronet also participates in the latest initiatives building EOSC: FAIRCORE4EOSC, EuroScienceGateway and EOSC Beyond. In the first project, our role is to provide expert support in the field of data management and personalised search of EOSC resources (including scientific objects) using AI methods. As part of EuroScienceGateway, Cyfronet is responsible for integrating the solutions of the Onedata distributed data management platform with the project infrastructure being built. In EOSC Beyond, Cyfronet is responsible for providing expert support and solutions for scientists in the field of new EOSC functionalities.

EuroHPC – European Data-Processing Infrastructure

The European High-Performance Computing Joint Undertaking (EuroHPC JU) was established to radically develop the existing European HPC infrastructure so that it could provide European researchers with computing power comparable to the ones available in the USA, China and Japan. EuroHPC unites 34 countries, from 2018 including Poland, as well as private members. The joint aim is to buy and deploy two exascale supercomputers (EFlops = 10^{18} floating points per second) that will be on the TOP5 list of the world's fastest computers.

The first European exascale supercomputer is JUPITER at the Jülich Supercomputing Center in Germany, which became the fastest European machine when fully installed in 2024. The second supercomputer with a power exceeding 1 EFlops will be located in the TGCC computer centre in France. Before that, however, subsequent lower-power supercomputers are launched, creating an infrastructure that allows the technology and software to be scaled. By the time this publication was prepared, EuroHPC JU had delivered 3 pre-exascale supercomputers: LUMI (Finland), Leonardo (Italy), Mare Nostrum 5 (Spain). Additionally, 5 petascale supercomputers were successfully put into operation: Discoverer (Bulgaria), Karolina (Czech Republic), MeluXina (Luxembourg), Vega (Slovenia) and Deucalion (Portugal). The next in this class of computers will be Daedalus (Greece). EuroHPC JU also finances the purchase of quantum computers. Polish scientists will have access to one of them, installed in the Czech Republic, via the PLGrid infrastructure coordinated by Cyfronet.

More about EuroHPC JU at: *https://eurohpc-ju.europa.eu/*.

Karolina Supercomputer, Czech Republic. Image: EuroHPC JU

Vega Supercomputer, Slovenia. Image: Atos

National Competence Centre in HPC

ACC Cyfronet AGH is coordinating the activities of the Polish National Competence Centre in HPC.

The National Competence Centres (NCC) were established as part of the European High-Performance Computing Joint Undertaking (EuroHPC JU). The EuroHPC JU was established to develop, deploy, expand and maintain Europe's world-class supercomputing and data infrastructure. The joint activities are intended to support the development of innovative technologies in Europe and increase the use of HPC (High-Performance Computing) infrastructure by academic users, governments and entrepreneurships in Europe.

In this light, the NCCs, funded through a series of EuroCC projects, are to serve as focal points for HPC and related technologies in their respective countries. They aim to improve and equalise European advanced computing capabilities and provide access to infrastructure and expertise.

EuroCC Poland is based on the partners of the PLGrid Consortium (ICM, PSNC, WCNS, CI TASK, NCBJ), whose leader is ACC Cyfronet AGH. The main tasks of the National Competence Centre include:

- supporting stakeholders from industry, the public sector and academia in the implementation of HPC technologies,
- increasing the use of HPC technologies among SMEs to raise their innovation potential,
- improving the visibility of existing HPC centre offerings and services for SMEs and industry,
- expanding the training portfolio,
- creating a catalogue of services that includes offerings from HPC centres and other key HPC services and technologies from vendors in Poland,
- raising awareness among various stakeholders, including Centers of Excellence (CoEs) and European Digital Innovation Hubs (eDIHs) in Poland and abroad.

Representatives of NCC Poland during the EuroHPC Summit 2024. From the left (in the second row): Marek Magryś, Cyfronet; Mateusz Tykierko, WCSS; Mariusz Sterzel, Cyfronet; (in the first row): Marta Maj, Cyfronet; Szymon Mazurek, Cyfronet

Details on the activities of the National HPC Competence Centre can be found on a dedicated webpage: *https://cc.eurohpc.pl*

The LUMI supercomputer

LUMI – No. 3 in Europe, No. 8 in the world

In November 2024 the subsequent TOP500 list of supercomputers with the highest computing power in the world was announced.

The LUMI supercomputer installed in the CSC data centre in Finland took the eighth place there and the third position in Europe. This undoubted success in the HPC (High-Performance Computing) environment is the result of the cooperation of 11 countries, including Poland, which form a consortium operating under the wings of a larger initiative, the EuroHPC Joint Undertaking. Importantly, thanks to the activities coordinated by ACC Cyfronet AGH and the Ministry, Poles have already gained access to LUMI resources.

LUMI among the world leaders in computing power and energy efficiency

Together with other petascale and pre-exascale systems in which EuroHPC JU is involved, LUMI is a part of the pan-European infrastructure to which fully exascale computers will also be incorporated in the coming years. Obtaining a place at the TOP10 of supercomputers is a great success for European countries because it shows the possibility of competing with systems from the USA, China and Japan. In High-Performance Linpack (HPL) tests, the LUMI supercomputer showed an actual power of 375 PFlops and a theoretical performance of up to 550 PFlops. This performance is made possible thanks to the LUMI hardware architecture:

- the GPU partition is composed of 2560 nodes, each of which contains a 64-core AMD Trento processor and four AMD MI250X cards,
- a single MI250X card can deliver 42.2 TFlop/s of performance in High-Performance Linpack tests,
- each GPU node contains four 200 Gb/s network connection cards,
- the addition to the GPU partition is the CPU partition, which uses the 3rd generation AMD EPYC™ 64-core general purpose processors.

However, during the design and construction of the LUMI infrastructure, a strong emphasis was put not only on the computing power, but also on the efficient use of energy. For this reason, the LUMI supercomputer also took the high, 25 place on the Green500 list of supercomputers with the highest energy efficiency, calculated as the ratio of computing power to electricity consumed. In addition, it is worth emphasizing that 100% of the LUMI's power supply comes from renewable sources (hydroelectric power plants), and the waste heat removed from the machine is used to heat the surrounding buildings. Thus, LUMI is now a flagship European example of implementing the idea of sustainable development in the construction of supercomputing systems.

More information about LUMI at: *https://lumi-supercomputer.eu*.

The representatives of ACC Cyfronet AGH during the inauguration of LUMI.
From the left: Mariusz Sterzel, Head of the Quantum Computing Laboratory and Marek Magryś,
Deputy Director of ACC Cyfronet AGH for HPC at that time

Access to LUMI for Polish scientists

ACC Cyfronet AGH coordinates work related to providing Polish scientists with the resources offered by LUMI. The aim is to ensure an efficient and user-friendly environment for working with a supercomputer, based on good practices developed within the PLGrid infrastructure.

In the period from autumn 2021 to spring 2022, Cyfronet organised two competitions for pilot computing grants on the LUMI supercomputer for Polish scientists. During the infrastructure testing period, 5 Polish projects were implemented. Subsequent competitions have concerned regular, annual access to infrastructure. Based on them, by the time of this publication's submission, calculations with the use of LUMI have already been carried out by 31 Polish projects. Access is provided via the PLGrid Portal (*https://portal.plgrid.pl*), and additional information is available at *https://cyfronet.pl/lumi*.

The project aims to provide a new alternative to open science and tools for science in the European Open Science Cloud (EOSC) context by giving a new EOSC Core platform feature. The planned improvements are intended to enable scientific applications to find, compose, and access open science resources and offer them as integrated solutions.

The main goal of the project is to provide an open and fully operational FAIR EOSC ecosystem. The project aims to expand the EOSC infrastructure with components supporting the FAIR paradigm (Findability, Accessibility, Interoperability, Reusability).

The aim of the project is to define and develop a new and innovative European Master's degree program focusing on HPC. The program is designed to equip students with HPC competencies and knowledge required by academia and industry.

Through the development of the EOSC Portal, the project aimed to extend the EOSC ecosystem, integrate existing scientific infrastructures and initiatives, and engage new domain and national research communities.

The main aim of the project was to deliver transparent and unified access to Earth Observation Data, primarily satellite data, in order to support food production and the food and agriculture industry.

The goal of the project is to create a computational medicine centre in Krakow. The Centre will be the main driver of European progress in this fast-growing sector, developing advanced engineering methods for the prevention, diagnosis, and treatment of diseases and meeting the global need for radically improved healthcare systems.

The aim of the project was to expand the computing infrastructure, enabling cooperation in the area of high-intensity problems connecting large volumes of data that cross the boundaries of a single data center.

The purpose of the EPOS-SP project was to develop and implement assumptions to ensure the sustainability of the EPOS infrastructure produced in previous projects (EPOS-PP and EPOS-IP).

The goal of the PRACE-6IP project was to implement new solutions and maintain the operationality of the PRACE environment in the area of European HPC computing infrastructures

The project aims to enable small and medium-sized enterprises (SMEs) and start-ups in Europe to conduct experiments using High Performance Computing (HPC) infrastructure and artificial intelligence (AI) methods to improve their competitiveness and innovation potential.

The mission of the project is to continue the creation of the EuroHPC National Competence Centers (NCCs) network in Europe through cooperation, exchange of best practices and knowledge, and upgrading the national and European levels of HPC service delivery.

The main objective of the project is to establish support activity for EuroHPC user applications at Level 2 and Level 3. As part of the project, an Application Support Team (AST) will be established, whose main task will be to cooperate with the EuroHPC JU application evaluation office and directly support projects that have obtained computing time on EuroHPC JU resources.

The project aims to build the science-based technology solutions needed to power Europe's next generation of video conferencing platforms and support and facilitate business collaboration across the European Union.

The aim of the project was to build a specialized general-purpose infrastructure for large-scale computing, enabling the undertaking of research challenges in key areas from the point of view of Polish society, the scientific community, and the economy. The project was the Polish stage of development of the EuroHPC program.

The goal of the project was to develop and provide production services for storing, accessing, securing data and managing metadata, as well as integrating solutions for processing large and complex data volumes on the basis of a distributed e-infrastructure.

Within the project the construction of unique research laboratories based on the national PIONIER fiber optic network was realised. The main goal of the project was to build and make available platforms for research units, entrepreneurs and other entities interested in conducting scientific research and development works based on a new, nationwide research infrastructure.

The direct goal of the project was to create a specialized e-infrastructure for data processing, enabling the optimal use of specialized and new generation services to stimulate new areas of application in science, economy, education and social life.

As part of the project, the functionalities of the EPOS-PL research infrastructure were increased. A new Research Infrastructure Center (Center for Research Infrastructure of Satellite Data – CIBDS) was established, a new test site (Geophysical Safety System for mining protection pillars) was created, and the WNiP was established: „IT Platform for Research with Artificial Intelligence Methods (EPOS-AI)".

The goal of the project was to create computing infrastructure services and data storage services for the purposes of the PRACE project, within six dedicated laboratories: 1) L. of HPC and cloud processing, 2) L. of access to processing infrastructure, 3) L. of service management and monitoring, 4) L. of data management services, 5) L. of distributed data management and transparent access to data, 6) L. of infrastructure security.

The main objective of the project was to provide satellite data coming from the Sentinel satellites of the Copernicus network. The project created an infrastructure for automatically downloading data directly from satellites, its secure storage and sharing for the purposes of science, administration and training.

The project aimed at building the national research infrastructure for solid Earth Science and its integration with international databases and services implemented under the European Plate Observing System (EPOS).

The objective of the project was the development of the specialized technological competence centre in the field of distributed computing infrastructures, with particular emphasis on grid technologies, cloud computing and the infrastructures supporting calculations on large data sets. As a result, great computing power and huge storage for digital data were offered to users. They also obtained access to a set of basic and end-user services.

The project aims to provide a quantum critical distribution infrastructure and a quantum communication network using the existing fibre infrastructure of the PIONIER network.

The project built a cloud environment for content from the CH (Cultural Heritage) area, processing and collecting high-quality content, allowing the launching of virtual spaces for an interdisciplinary and cross-sector community cooperating with the CH area.

The project will provide new or significantly improved access to key observations, data products, and services that enable the monitoring and simulation of dynamic processes in the geosphere at an unprecedented level of detail and precision, both spatially and temporally.

The laureates of previous editions of the Contest

Work of young scientists in Cyfronet

The annual contest for the best PhD thesis conducted with the help of computing resources of ACC Cyfronet AGH is a tradition in our Centre. The scientific value of the submitted doctoral dissertation is assessed, as well as the possibility of its practical application and the scope of use of computing resources and disk storage in Cyfronet. In recent years, the Contest has become an important event promoting research conducted by young scientists. To subsequent editions of the Contest, participants submitted many PhD theses focused on various scientific problems in chemistry, biophysics, physics, and computer science. Also, the utilisation of the resources varies, as the contesters use different tools running on a wide range of computing architectures offered by Cyfronet.

The laureates of the Contest are invited to give a talk during Cyfronet's Open Day. We are honoured to present here selected interviews with the Contest participants.

Join the next Contest edition!
http://www.cyfronet.pl/konkurs

The laureates of the Contest in 2024

Andrzej J. Kałka, PhD

Jagiellonian University in Krakow

The interview with the author of the PhD thesis:
"Development and Implementation of Computer-Aided Techniques of Data Modeling for Processing and Interpretation of Multicomponent Electronic Spectra Acquired for the Selected Organic Mixtures"

How did you become interested in chemometrics?

This may sound somewhat cliché, but it was mainly due to my Supervisor. Early in my studies, I realised that the issues typically associated with chemistry, such as synthesis or analysis of specific samples, did not arouse much enthusiasm in me. Far more fascinating to me seemed (and still seem) to be the issues involved in discovering and describing the nature of the phenomena to which these samples might be subjected and through which they came into being. This conviction threw me straight into the arms of physical, theoretical and computer chemistry. In a strict sense, I was introduced to the arcana of chemometrics as part of my undergraduate work. Although this subject initially appeared to me somewhat abstract, I soon learned that the proper use of mathematical apparatus and computer technology makes it possible to extract information from data obtained in chemical measurements that is not available to „mere mortals." Captivated by this prospect, as part of my scientific work, I decided to devote myself to developing this methodology and its practical application, which, as I have unfortunately experienced many times, is still rare.

What determined the choice of the MATLAB package as one of the primary computing environments used in the study?

In a sense, I didn't have much choice in the matter – the chemometric environment took a liking to this package quite early in its development. Hence, MATLAB naturally became (and remains), so to speak, the default choice for conducting chemometric calculations. With the benefit of hindsight, I reaffirm my conviction that this choice remains quite correct. After all, the core of most algorithms is linear and matrix algebra calculations, for which MATLAB (short for MATrix LABoratory) was created, thus offering a considerable amount of dedicated functional solutions. In addition to the console, the package also has a built-in graphical interface (GUI), which – compared to, for example, the R package – significantly facilitates the processing and visualisation of data, including, for example, the creation of complex, multi-element graphs.

What were your most significant difficulties on your research path, and how did you face them?

The problem that thwarted my (and probably not only my) plans to the greatest extent was the SARS-CoV-2 pandemic, coinciding with the first two years of my doctorate. At that time, national and international research exchanges were virtually completely halted, preventing me from attending internships, training courses or conferences. Fortunately, the imposed restrictions did not significantly affect the implementation of my research – the computer technology I primarily based it on proved resistant to the coronavirus and found itself well in the new „remote" reality. The second problem, which I believe is worth to be mentioned publicly, was the difficulty in obtaining funding to conduct my research. Unfortunately, the pool of grants intended to fund projects authored by young scientists is, to put it mildly, not one of the largest. Thus, obtaining funds for their implementation is often very hard or even impossible. In my case, the „Initiative for Excellence – University Research" (IDUB) program proved to be very helpful, within the framework of which, in the form of so-called mini-grants, support was given to projects submitted precisely by doctoral students.

Concerning the posting of the developed algorithms in the RODBUK database, how do you assess the validity and need to publish the data in open access?

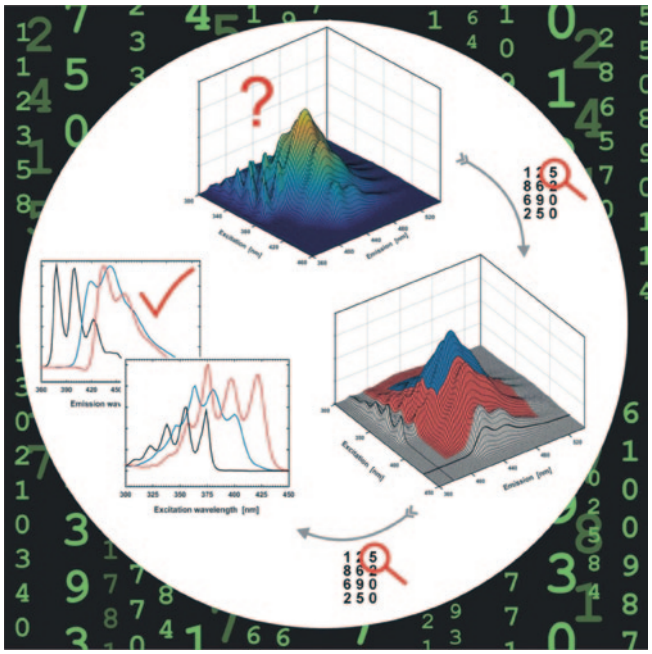
The initiative of so-called „open science" seems very right in principle. In my opinion, the results of reliably conducted research, in general, should be widely available to all interested parties. Unfortunately, the problem is the practical implementation of this assumption. Publishing in the „Open Access" (OA) format is associated with quite significant costs (on the order of several or even several thousand PLN), which a large number of scientists simply cannot afford to cover. Therefore, it is only possible to applaud the idea of open data repositories (such as the cited RODBUK), in which materials related to ongoing research can be deposited free of charge and then made available to a wide range of potential recipients.

To what extent have the IT resources provided by Cyfronet benefited the research being conducted?

While modeling experimental data using an „ordinary" computer should not pose significant problems in practice, I cannot imagine conducting quantum-chemical calculations with its help, which are an essential part of my research work. For example, to obtain the result of one of the typical simulations (of which I have performed dozens, if not hundreds, as part of my doctorate) on the Ares supercomputer I needed a little over two hours – the same simulation on an average PC would have taken me an estimated half a day. Given the above, I can, in good conscience, describe the computing resources provided as invaluable. Presumably, my opinion will also be shared by dozens of other users of the PLGrid infrastructure, with whom – especially recently – it fell on me to compete for a place on the podium in the slurm queue system.

What would you advise budding scientists starting or planning to start doctoral schools?

Above all, they should think honestly about their motivation and priorities. The PhD studies, especially under the current law on education (doctoral schools), offer a significant number of opportunities for scientific and personal development. However, to take full advantage of these opportunities, which, of course, I strongly encourage you to do, you need to have enough time, and this can be carved out only at the expense of reducing or even abandoning regular gainful employment. This, in turn, may reflect negatively on your work experience and, consequently, your position in the labour market (outside the R&D sector) immediately after completing your doctorate. It is therefore necessary to honestly answer whether, from the perspective of the next four years, scientific or professional development is more important to me. At this point, it is worth mentioning in a buzzword the program of so-called „implementation doctorates," offering, in a sense, a middle option between the two extremes above.



Chemometrics – what it is all about?
A scheme taken from A.J. Kałka, A.M. Turek (2021), J. Fluoresc. 31: 1599-1616

Damian Kułaga, PhD

Cracow University of Technology

The interview with the author of the PhD thesis:
"Study on discovery of novel 5-HT_{1A}/5-HT_7 receptor ligands acting on the central nervous system, in the group of long-chain arylpiperazines and aminotriazines"

What made you interested in chemistry, both in experimental and computational aspects?

My interest in chemistry (or, in fact, life science) goes back to fairly early adolescence, when, as a teenager, I performed simple experiments and thus learned chemistry and how life on Earth is structured. High school and college oriented me more and more toward medicinal chemistry. At the same time, the most significant leap in my knowledge came when I took a job at a biotechnology company in Krakow. There, I learned the ins and outs of organic chemistry and how it can be applied to drug design. Also there, I made my first contact with the actual drug discovery process and the application possibilities of computational chemistry in this field. It turns out that you don't need to synthesise large libraries of compounds and then test their performance. It is possible to harness a computer to show which direction a chemist should take synthetic action and which group of compounds is not worth synthesising in the context of a particular biological action. This significantly reduces the effective working time of the scientist and, moreover, reduces the cost of the entire scientific project. Having the basic knowledge, I decided to develop it in my research conducted during my doctoral studies.

Under what circumstances did you decide to devote your doctorate to designing compounds with specific pharmacological effects?

As I mentioned before, the nature of my professional work prompted me and instilled in me the desire to conduct my research. I wanted to experience scientific success, verify a given research hypothesis, and experience the taste of failure. By a stroke of luck, my PhD supervisor at the time obtained a research grant funded by the National Center for Research and Development, and a full-time position appeared within the framework of this grant. Of course, without hesitating, I took the opportunity. An additional consideration was that the project involved the development of compounds that exhibit biological activity on serotonin receptors so I could further hone my medicinal chemistry skills and develop an interest in computational chemistry. We know that diseases of the central nervous system (such as depression and ChAD) right after cancer and heart disease are some of the most common causes of death. For this reason, I wanted to contribute (even if only slightly) to developing drugs or agents that could become medicines to help those ill.

Why is it essential to seek ecological methods of synthesising new compounds? How do you assess your activities in this area?

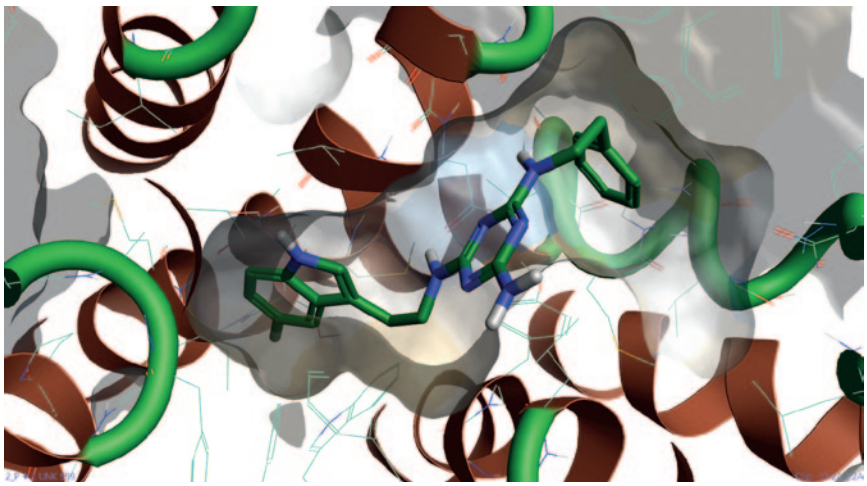
This is important for several reasons. First of all, the new synthesis methods allow for better environmental protection, and it is known that the European Union is strongly betting on measures in this

area. Another key reason is to save money. By better optimising processes, reducing, for example, synthesis time, the number of solvents used, the amount of waste generated, or improving atomic economics, a significant amount of money can be saved. In addition, the COVID-19 pandemic has highlighted, as if through a lens, how vulnerable the raw material supply chains are, whose base is mainly in Far Eastern countries or India. Being able to synthesise in one's home country (or even in EU countries), but based on environmentally safe technologies will make it possible to become independent of Asian countries, where, as it is well known, ecological issues are treated with neglect. Thanks to the work I carried out during my doctorate, I significantly reduced the time for synthesising compounds from as much as several tens of hours to as little as 2.5-5 minutes. Reactions were carried out solvent-free or in the presence of water alone. As a result, I conducted the syntheses in an environmentally safe, low-cost, and efficient manner, reducing the carbon and water footprint as much as possible.

How did the resources offered by Cyfronet help with the research?

The resources offered by Cyfronet helped primarily in the design of new molecules. Using the Prometheus supercomputer's computational power, I could perform studies related to docking and molecular dynamics for new molecules. This work showed which fragments of molecules are responsible for biological activity and which chemical group had to be selected for further synthetic work. These studies would not have been possible with an "ordinary" computer due to insufficient computing power.

What, in your opinion, should be paid special attention to by researchers just entering the path leading to a PhD defence?



Docked 5-HT$_7$ receptor antagonist in the binding site

For them to be resilient to adversity, of which there will be many. Often, a scientist's work is arduous and does not always lead to the expected results. This can be demotivating. Naturally, a given experiment will not work out, but this is also a clue for young scientists as to what they should do better to make the work successful. The aforementioned tediousness of the work means that such a person may spend many hours in the laboratory and even more hours at home, designing new experiments or searching for information in the literature (if they are ambitious). In my opinion, one cannot overdo it; a young person must maintain a "work-life balance" because without this, unfortunately, there is a risk of professional burnout, often making it difficult or even impossible to defend a doctorate. One more important thing that a young scientist should pay attention to is making friends and establishing national and international collaborations. Working together opens up opportunities for valuable interdisciplinary research, the formation of scientific consortiums, and potential research or post-doc positions.

Photo: Jan Zych, PK

Izabela Kurzydym, PhD

Cracow University of Technology

The interview with the author of the PhD thesis:
"Modeling of catalytic reactions in the deNOx and deN_2O processes by Selective Catalytic Reduction"

What was behind the decision to devote the doctoral thesis to processes related to reducing nitrogen oxides?

Ecology in science is currently being discussed in almost every case. As a resident of Krakow, I experience the phenomenon of smog daily. I wanted my dissertation, which I was to devote several years to, to have an impact on improving the quality of life. The possibility of studying more efficient catalysts in reducing nitrogen oxides, i.e., compounds that are part of air pollution, seemed incredibly interesting. Working out the mechanisms and discovering the correlations, but also the differences, gave me immense satisfaction. For more than 30 years, the European Union has been introducing increasingly stringent directives on gas emissions to make our air cleaner and our lives more comfortable. Therefore, I hope that the scope of my research will positively impact the development of new technologies for cleaning waste gases in the industry, especially the nitrogen industry, which is essential for producing fertilisers.

How could you briefly introduce readers to zeolite catalysts and their potential for implementation?

Zeolites are crystalline structures consisting of silicon, oxygen, and aluminum atoms, sometimes with the addition of other metal atoms if the zeolite comes from natural sources. Due to their porous structure, they have a large specific surface area, which allows them to quickly deposit, for example, transition metals inside the pores, which in turn provide active catalytic centres. In addition, zeolites are characterised by thermostability and lack of toxicity, which significantly facilitates their use in industrial processes, often occurring at high temperatures. Moreover, for reactions in which the reactants are in the liquid or gaseous state, the ease of separation of the zeolite catalyst from the product is of significant industrial importance.

In light of your work and a broader context, how do you assess the validity of computer modeling of industrial processes?

I can cite an anecdote here. In my work, I conducted calculations for nitric oxide reduction with ammonia, which can co-occur with nitric oxide reduction with nitrous oxide. At one conference, a clinoptylolite zeolite that I had studied was presented, which had been implemented in an industrial plant to reduce nitrous oxides in waste gases in the nitric acid production process. The researchers showed a reduction in nitric and nitrous oxide concentration in the waste gases, but they did not understand the latter phenomenon. Thanks to my calculations, I was able to show the mechanism that affects the reduction of nitrous oxide concentration and help them understand the catalyst processes. This shows the importance of conducting combined experimental and theoretical research that can complement each other.

What have you used Cyfronet's resources for, and to what extent?

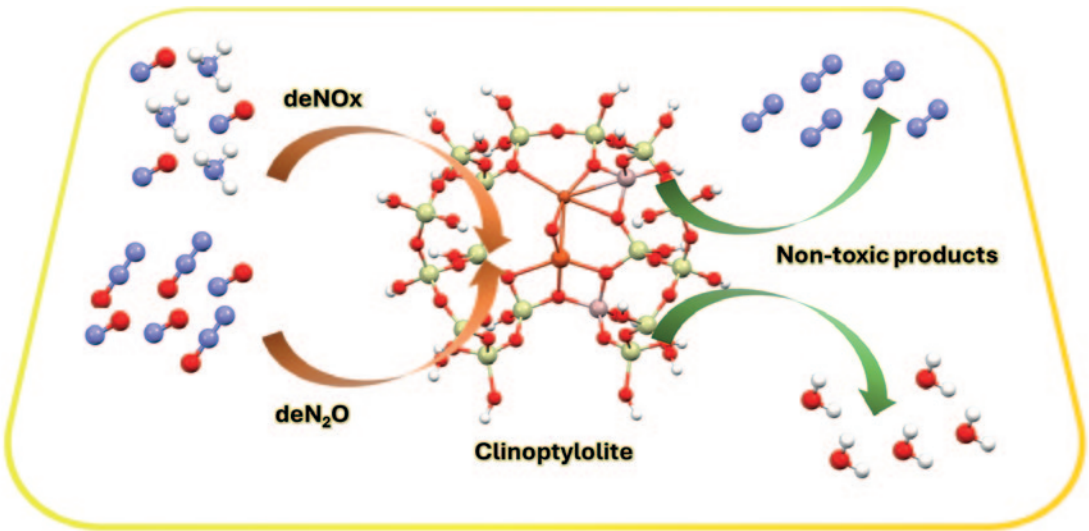
The resources of the Cyfronet's supercomputers allowed me to run multiple calculations simultaneously. Thanks to the high computing power, I could easily conduct calculations for structures consisting of many atoms and receive results for analysis in a relatively short time. In my dissertation, I included 72 diagrams describing the mechanism of deNOx and deN_2O. This required thousands of individual calculations, which was only possible thanks to Cyfronet's resources. I also had the opportunity to see

how rapidly the supercomputing infrastructure at Cyfronet is developing. I am continuing my scientific career using the resources of the new Ares supercomputer, and I am looking forward to testing Helios. It is great to see the development of the infrastructure, which translates into increased efficiency for researchers. I am very grateful for the opportunity to use Cyfronet's resources.

What would you advise researchers at the beginning of their scientific journey? What would you encourage them to do?

I sometimes think that computational chemistry inspires a particular fear among young scientists. It doesn't seem very easy and not very approachable. However, it is essential not to be discouraged by the subject. Today, chemistry and science are developing towards using computational methods or artificial intelligence to help us deeply understand the world around us. So it is worth at least minimally including computational chemistry in your work, if not conducted independently, then through collaboration with other scientists.

Young scientists should also keep an open mind and listen to good advice from more experienced scientists. However, it is worth remembering to be bold and talk about your innovative ideas. Setting your main career path as a scientist is a good idea. Still, it's important to consider that there are many exciting paths away from it, which are worth entering at least for a while to enrich our knowledge of the macro, micro, and quantum world.



Schematic representation of the combined deNOx and deN_2O process on a clinoptylolite catalyst

Sabina Lichołai, MD

Jagiellonian University Medical College

The interview with the author of the PhD thesis:
"MicroRNAs as potential biomarkers of abdominal aortic aneurysms"

In a non-specialist way, how would you characterise the identification of molecular profiles associated with abdominal aortic aneurysms?

The process of identifying molecular signatures associated with vascular disease can be divided into two main steps: performing high-throughput molecular experiments and executing computational analysis. Each stage is crucial to obtaining a complete molecular profile of the patient and is of great diagnostic importance. The first step involves using modern molecular biology techniques, such as next-generation sequencing (NGS), proteomics or metabolomics. These techniques allow us to examine thousands of genes, proteins and metabolites in patient samples simultaneously. With these technologies, we are able to obtain a detailed molecular profile that shows what changes are occurring at the genetic, protein and metabolic levels in the bodies of people with vascular disease. The second stage is advanced computational analysis. Once we have the raw molecular data, we use bioinformatics and statistical tools to integrate, process and interpret the data.

What is the significance of your research in diagnosing and treating patients with this disease?

Among other things, our analyses include comparing the molecular profiles of patients with controls to identify critical biomarkers and develop predictive models. These models can help predict disease course and response to treatment. Combining the two research layers I mentioned earlier allows us to obtain comprehensive molecular profiles of patients that can be used to diagnose and personalise therapy. It also allows us to more accurately understand the mechanisms underlying various disorders, such as vascular disease, which may lead to more effective treatment strategies in the future.

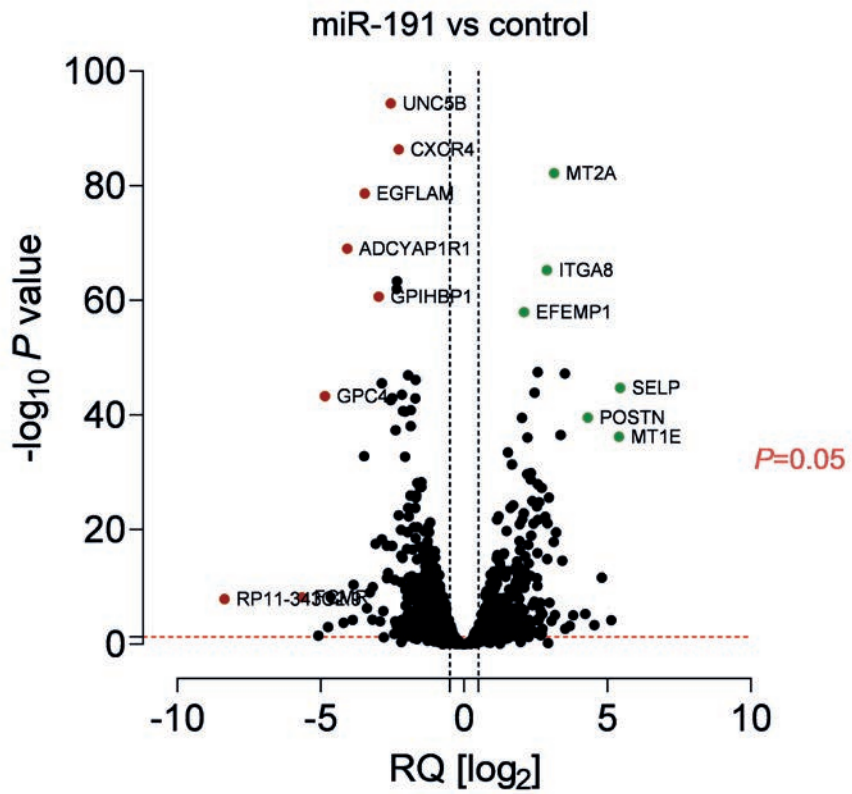
Can you comment on the need – but also the potential – of modern diagnostic development based on IT tools?

Traditionally, molecular diagnostics has focused on analysing proteins, which are direct effectors of many biological processes. Methods such as ELISA, western blotting, and mass spectrometry were commonly used to identify and quantify proteins in biological samples. While these methods have provided a wealth of valuable information, the search for new biomarkers with their use seems to be slowing down, and the pool of protein products is also limited. Non-coding nucleic acids, such as microRNAs (miRNAs), long non-coding RNAs (lncRNAs) and other small non-coding RNAs, are a promising new direction in diagnostics. NcRNAs play a crucial role in gene regulation and are associated with many disease processes, making them potentially valuable diagnostic biomarkers. Identifying and analysing ncRNAs requires advanced technologies such as high-throughput sequencing (NGS

– *next-generation sequencing*). NGS enables simultaneous sequencing of millions of DNA or RNA fragments, which is crucial for discovering new biomarkers in large and complex data sets. On the other hand, high-throughput sequencing generates vast amounts of data that must be efficiently analysed and interpreted. This is where advanced computing tools or infrastructure, such as computing clusters and dedicated bioinformatics algorithms, come onto the scene to process such large data sets efficiently.

How, in the above regard, have the resources of the ACC Cyfronet AGH benefited your research?

ACC Cyfronet AGH allows Polish scientists to perform research using computing clusters. The computing power provided is necessary to perform the required analyses due to the vast amount of data generated, the complexity of the analyses and the need for fast processing. Performing such procedures is impossible, for example, based on typical laptops or computers designed for gaming. Besides, large amounts of data require not only computing power, but also appropriate systems to store and manage them. The infrastructure offered by Cyfronet here provides scalable solutions for storing and processing large-scale data for scientific research.



Alterations in gene expression at the transcriptome level due to epigenetic factors

What do you think students should keep in mind at the beginning of their doctoral path?

Above all, I would emphasise the importance of choosing the right research topic. It should be an area that, on the one hand, interests us strongly, but also represents a niche in the field. In doing so, it is worth looking at interdisciplinary research directions that combine even significantly different fields. Such an approach can lead to innovative solutions, allowing us to look at a problem from different perspectives and use methods and tools from different disciplines. It is also worthwhile to attend scientific conferences and industry meetings at an early stage. It allows you to make valuable contacts, exchange experiences, and stay abreast of the latest trends in your field.

Karol Ławniczak, PhD

University of Lodz

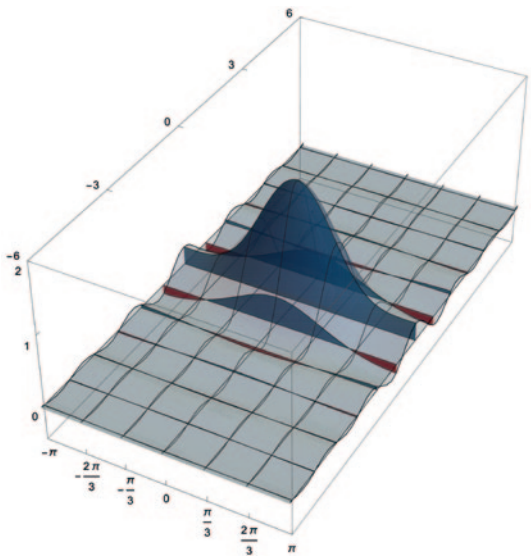
The interview with the author of the PhD thesis:
"Wigner function on topologically non-trivial manifolds"

How has your interest in quantum mechanics developed?

My interest in quantum mechanics is nothing more than an interest in how reality works. The same interest drives kids to explore the world and ask that annoying "why" question. It just hasn't gone away for me. Naturally, it is the natural sciences and their philosophical "background" that seek to answer such questions. Physics deals with the foundations of how reality works, so it requires more profound reflection but gives the most satisfying explanations. That is probably why my main field of interest is physics, particularly fundamental physics (although I have also dealt with research in other areas, amongst them riverine ecology).

What made you decide to devote your dissertation to the Wigner function? What distinguishes your approach in light of previous research?

In classical physics, a particle simultaneously has a well-defined position and momentum so that its state is represented by a point in phase space. For a statistical ensemble of such particles, the probability of finding one in a given region of phase space is described by a joint probability distribution. In quantum mechanics, the Heisenberg uncertainty principle precludes the simultaneous exact determination of the position and momentum of a particle. Therefore, it is impossible to formulate a probability distribution on phase space. The Wigner function is the closest analogue of such a distribution. Formulating the problems of quantum mechanics in a way that is close to the mathematical structure of classical mechanics makes it possible, amongst other things, to:



Wigner function of the coherent state on a circle as a function of the continuous angular variable and the discrete angular momentum

- recognise which of the properties of quantum mechanics that distinguish it from classical ones are physically relevant properties of the theory and which are artefacts of a different mathematical formalism;
- conveniently study the behaviour of quantum systems while going over to the classical limit;
- not to give up certain intuitions formed as a result of dealing with classical physics.

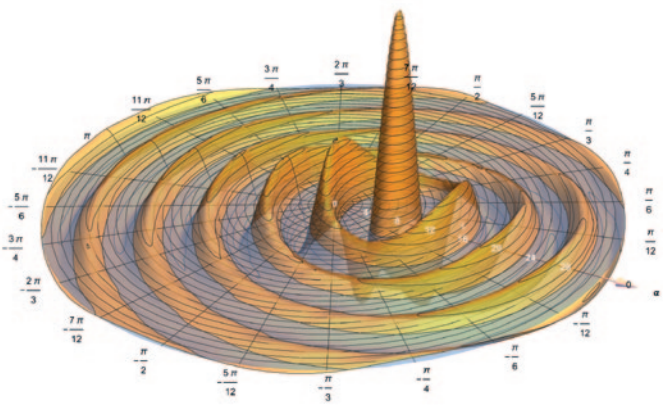
Definitions of objects and tools of quantum mechanics on phase space have been constructed under the assumption that a system's configuration and phase spaces are topologically equivalent to Euclidean space. Meanwhile, such a natural and vital issue as the study of rotational degrees of freedom of quantum systems, e.g. in atomic and molecular physics, requires the involvement of topologically non-trivial manifolds since the angles of orientation on a plane and in space belong to the circle and the sphere, respectively – certainly non-trivial manifolds, and non-trivial in different ways.

What were the most significant challenges on your research path?

The biggest challenges in my research work were the conceptual difficulties involved in generalising objects defined in Euclidean space to topologically non-trivial cases. Suffice it to say that the very notion of average has to be thought through when the variable being averaged belongs to a topologically non-trivial domain. Let us try to write down the formula for the mean wind direction and test it for a set of three data points (azimuths): 1°, 359°, and 180°. Even such a simple example requires concepts of statistics on the manifolds: the extrinsic mean or, in a sense, better, though less known, the intrinsic mean. And saying that expectation values play an important role in quantum theory is like saying nothing. There are more difficulties of a similar nature (albeit less apparent and more nuanced), and many of them have not had a satisfactory solution. I am happy to say that I have been able to unravel and illuminate some of them sufficiently so we may treat them as explained. Another challenge was the numerical simulations, which proved to be more demanding than I had anticipated at the start of the work.

In this last aspect, how have you used the resources provided by Cyfronet?

During my research, it was necessary to perform numerous integrations over several variables, including integration over unbounded intervals, and to optimise functions involving such integrals. On top of this, the integrands were fast-varying functions, and they covered a wide range of positive and negative values, which cancelled out almost entirely, but still not to zero. Performing these calculations so that the result was sufficiently precise and, above all, reliable was computationally demanding. Fortunately, at least some of them could be parallelised effectively. Without HPC, completing them in a reasonable time would have been impossible. My calculations were performed on Ares computer using Mathematica software. I would like to emphasise that a lot more calculations had to be done than the part of them presented in the dissertation might suggest. Such is the nature of research work that one tries many approaches before finding the right way, at least when exploring a new area.



Wigner quasiprobability distribution for a coherent state with non-zero angular momentum on a sphere depicted in angular momentum space

What advice could people planning to start or just starting down the doctoral path get from you?

I would encourage them to worry less about the PhD and more about the research itself. If you have an interesting topic, you need to explore it, pursuing your passion for discovering reality, which, I hope, guides all scientists or adepts in Science. Such an attitude will make it enjoyable, and there is a greater chance that the results obtained will be valuable. Then, the degree (when we finally write the dissertation) will be gained, as it were, in passing.

Krzysztof Maćkosz, PhD

AGH University of Krakow

The interview with the author of the PhD thesis:
"Atomic structure and electron transport in nanostructures of canonical topological insulators"

What inspired you to devote your dissertation to the properties of bismuth chalcogenide nanostructures?

The miniaturisation of silicon technology is a significant step forward, but continuous development is constrained by inherent limitations. Combining nanofabrication with novel materials represents a significant opportunity for further technological advancement and marks a milestone in the field of quantum computing.

How can the results you obtained influence the development of devices based on topological insulators?

The world of nanotechnology is still uncharted territory. The methods used to fabricate nano-devices can significantly alter the physical properties of quantum materials. This is why I'm so passionate about research into atomic-scale materials and nanoscale fabrication techniques. It allows us to better understand these phenomena and discover new possibilities in the field of nanotechnology.

What in your scientific work gives you the most excellent satisfaction?

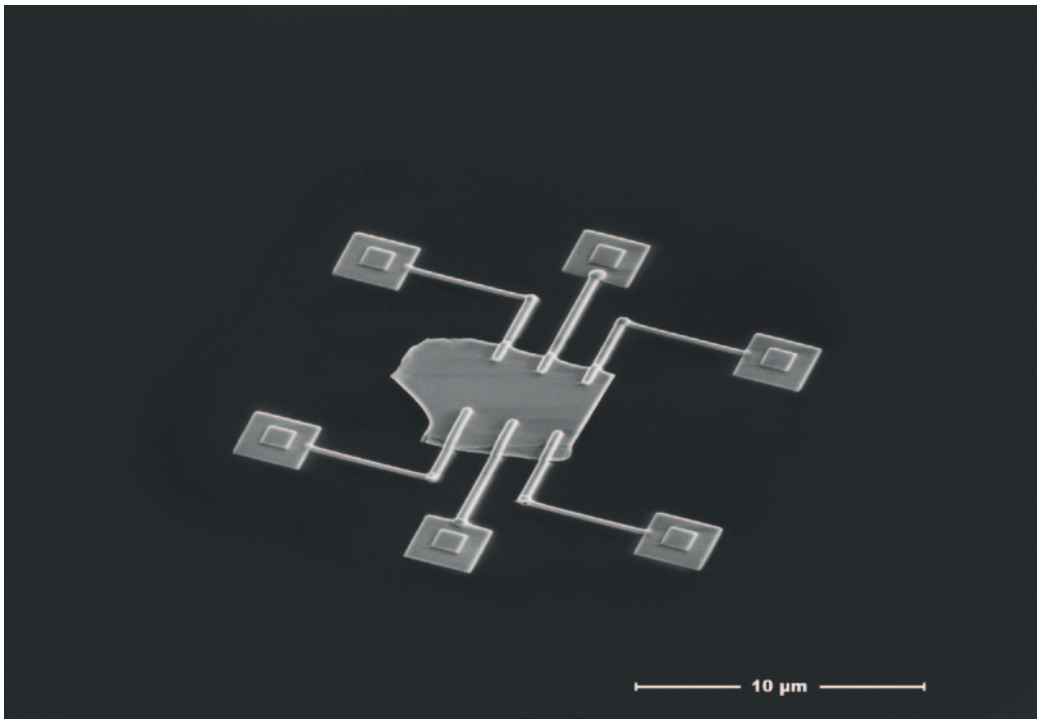
My greatest satisfaction in scientific work is derived from the exploration of the universe and the conduct of research, my tiny piece of the puzzle that contributes to the progress of technology. Above all, I value the opportunity to work with extraordinary people and brilliant scientists.

What resources provided by the Cyfronet were used in your research?

Many scientists see experimental and theoretical research as two distinct paths that never intersect. For me, the use of high performance computing for theoretical studies is crucial as it allows me to predict physicochemical properties, which is an essential complement to my experimental research.

If you were to give some brief advice to those planning to start or just starting a PhD program, it would be...

A PhD is a long journey through the unknown, filled with difficulties and challenges. One needs to know well what they are aiming for. Achieving the desired goal brings great satisfaction.



The crystal of a topological insulator, used to determine electron transport properties, obtained using a scanning electron microscope

Leszek Malec, PhD

Jagiellonian University in Krakow

The interview with the author of the PhD thesis:
"Experimental and *In Silico* Study of Polar Crystals"

Why did you decide to focus your research on intermolecular interactions in multicrystals?

The design of new materials for use in the different parts of the industry is nowadays a well-thriving part of science, which consumes enormous amounts of natural resources, money, and time. Therefore, the vast development of methods based on the planning of material structure at the sub-nanoscale has been observed. One of the most significant branches of designing multi-component crystal structures to obtain a material with a desired physical property is crystal engineering, which uses the understanding of intermolecular interactions in the context of crystal packing. The properties of crystals are not a simple function of the properties of the individual building blocks. Instead, they depend strongly on the interactions between molecules in the structure and their relative orientation and position. Thus, to create new materials rationally and efficiently, we need to know how they "work" on the atomic scale in currently known functional materials. The motivation for my research was to create a methodology based on quantum-chemical calculations and X-ray diffraction experiments to correlate the dynamics of interactions in a crystal with its macroscopic properties. In addition, each of the studied systems had features whose explanation had escaped the experimental methods used so far, which itself was an exciting research challenge.

What further research steps can be taken based on your results?

The applied methods and software can be adapted to study a wide range of physical properties in a broad spectrum of materials. The developed methodology enables the study of structural phase transitions and dynamic disorders occurring in crystalline phases. I hope that both my method of analysis and the results obtained will provide a better comprehension of dynamic structural transformations and the related macroscopic effects, thus enabling the engineering of new functional materials. An example would be ferrocaloric materials, such as the studied ammonium sulfate, which can be used to manufacture more efficient and environment-friendly cooling systems. The problem of the disappearance of a given crystalline phase is well-known in the pharmaceutical industry, generating huge losses when a given polymorph is used in drug production. The results obtained, explaining the disappearance of the polar polymorph of the urea-barbituric acid co-crystal, should allow a better understanding of this phenomenon and stimulate further research on the impact that in-solution pre-organization of molecules has on the crystallisation process.

In your paper, you mention the use of in-house software for analysing the dynamics of hydrogen bonding systems. Can you give a brief overview of the software?

The main objective of the prepared software was to analyse temporal and spatial correlations between changes in geometric parameters of molecules/ions in the studied systems. The software enables the analysis of dynamic disorder in the simulated crystal structure due to the individual study of the parameters for each ion, molecule, and bond within the computational cluster. Each calculated parameter can be averaged in time and space (including consideration of the space group symmetry), allowing comparison of simulation results with data obtained using an X-ray diffraction experiment. In the program, each molecule/ion is an instance of a selected class that stores the Cartesian coordinates of all atoms. This allows quick calculation of selected bond

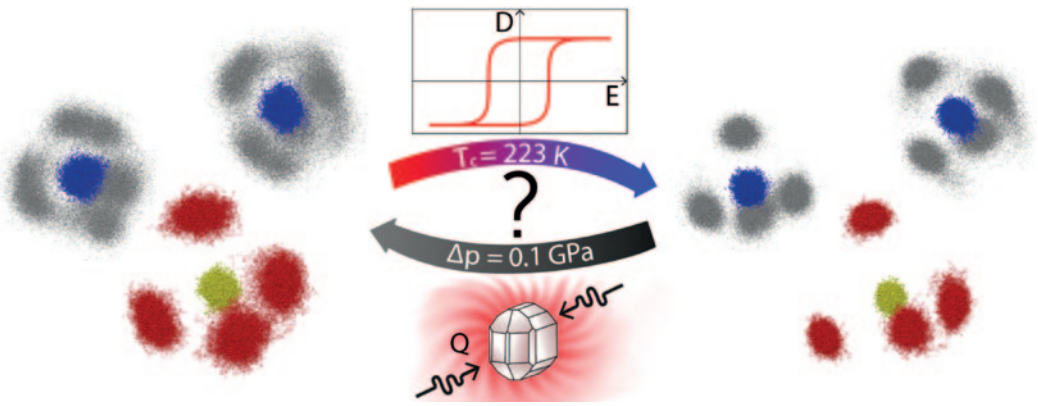
lengths, valence angles, and torsion angles for the selected molecule type. In addition, in some cases, I implemented the determination of more complex geometric parameters, including the volume of a molecule based on the determination of its convex hull. The entire computational part of the program was combined with a visualization module to automate the results' depiction.

How have you used the IT resources provided by Cyfronet?

Using the Ares and Prometheus supercomputers, I performed more than 70 simulations using the Born-Oppenheimer molecular dynamics method for several types of crystals in the CP2K program. Simulated clusters contained tens to thousands of atoms. In each case, the periodic boundary conditions were applied. Due to the size of the systems and the calculations' complexity, most of the computations used 288 to 432 cores. The obtained resources allowed vibrational analysis of each system using the generated power spectra and their decomposition. The obtained disk resources allowed me to analyse the intermolecular interactions in studied crystals utilising the in-house software discussed previously. In addition, for two studied systems, I performed the Energy Decomposition Analysis using several thousand selected geometries from the determined trajectories. For this purpose, I used the backfill method, requiring thousands of short jobs on the HPC cluster. The calculations allowed me to explain the mechanism of the phase transition in ferroelectric ammonium sulfate and describe the phenomenon of proton transfer in three-component crystals containing a polycationic chain motif. I also explained the phenomenon of the polymorph disappearance for the case of urea-barbituric acid co-crystals, which allowed me to develop an experimental method to obtain the polar form in a repeatable manner.

What advice could you give to those starting doctoral school?

Due to its unique nature, scientific work gives us much freedom in organising our time and what we want to do. In choosing our scientific subject, we should be guided primarily by what interests us and what our research can give to others. One should not be afraid of change and become attached to what one has dealt with in earlier stages of education. PhD studies give us time to develop our research skills, learn how to share our knowledge, and network with other researchers. It is up to our independent choices to make our work both rewarding and valuable. A lack of enjoyment in what we do can easily lead to a loss of curiosity, which, for me, has always been the primary motivation for doing research. Therefore, from the beginning of a PhD, we should be aware of why we want to pursue a particular topic and focus on those aspects of research that will help us develop scientifically.



Graphical representation of the phase transition in ammonium sulfate (reprinted from L. M. Malec et al. Acta Materialia, 2021, under CC BY 4.0)

Agnieszka Winiarska, PhD

Jerzy Haber Institute of Catalysis and Surface Chemistry PAS

The interview with the author of the PhD thesis:
"Tungsten aldehyde oxidoreductase from *Aromatoleum aromaticum* – biocatalyst for alcohol production"

How would you explain the subject of your research to a person unrelated to the field?

My research aimed to understand better the enzyme aldehyde oxidoreductase from the bacterium *Aromatoleum aromaticum* (AOR for short). In my work, I showed a new activity of AOR with potential practical importance – the reduction of carboxylic acids using molecular hydrogen as an organic reductant, allowing energy conservation, e.g., bioalcohol. These reactions occur in an active centre containing a tungsten ion bound in an organometallic complex. To solve the reaction mechanism of AOR in this unusual reaction, I had to study its structure in more detail, for which, in addition to cryo-electron microscopy, I also used molecular modelling methods.

Is it possible to single out a breakthrough moment in your research?

During the characterisation of AOR, I discovered its new activity as hydrogenase, which had never before been reported for tungsten enzymes. This means that AOR is capable of oxidising molecular hydrogen dissolved in water and uses the resulting electrons to reduce either carboxylic acids or electron mediators such as nicotinamide adenine dinucleotide (NAD). This discovery has directed my research on AOR to more applied aspects of biocatalysis, among others, using this enzyme in enzymatic cascades to synthesise valuable compounds.

An essential moment in my research was also the determination of tungsten coordination, thanks to the combination of structure studies by theoretical methods and electron microscopy of a single AOR molecule. The geometries of cofactor models with different possible tungsten coordination, optimised by cluster QM and QM:MM methods, were verified by comparison with the crystal structure of AOR from *P. furiosus* and cryo-EM. The study revealed the most likely structure of the oxidised tungsten cofactor.

Could you please present the applicability of the results of your research, especially in light of their patent applications?

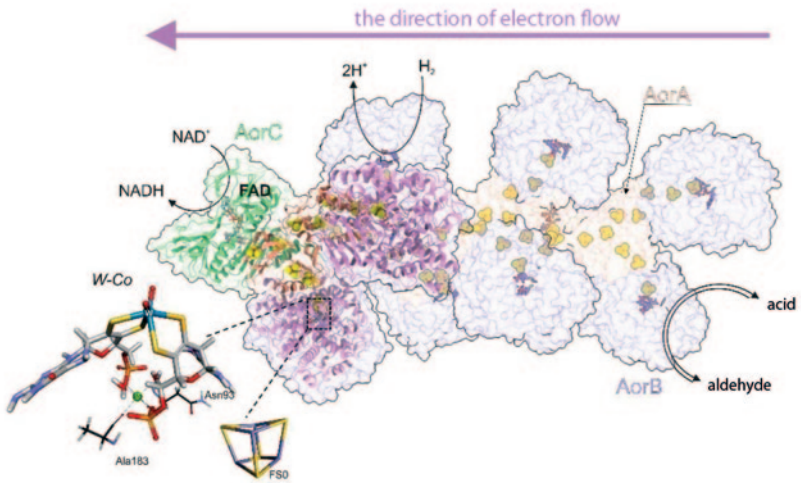
The activity of AOR as a hydrogenase can be used for energy conservation, e.g. in the form of bioalcohol, and in the clean and selective (no by-products) synthesis of aldehydes and their derivatives used in the food and pharmaceutical industries and in high-tech materials. Due to the selectivity of the acid reduction process and the clean method of NADH regeneration, AOR has excellent potential for use as a biocatalyst in new pathways for synthesising drugs, food additives (vanillin) and other valuable compounds. AOR also catalyses the oxidation of aldehydes, even at very low concentrations, which can be used in electrodes to detect or remove these often toxic compounds.

How do you assess the usefulness of Cyfronet's IT resources for supporting scientific research?

I believe that the Centre's resources provide the opportunity to conduct research at a level that competes with leading centres of this type. In my work, I have used many tools provided by Cyfronet i.e. for molecular modelling with QM and QM:MM methods, for protein structure analysis, and for molecular docking. The ability to use new versions of software such as Amber and Gaussian on supercomputers allowed me to study the tungsten cofactor in the largest, and thus, most accurate, optimised model of this type of cofactor to date and I must emphasise that many groups, including ones in the USA, undertook previous studies. Without such resources, the structure of the cofactor would continue to be a mystery, and it would be impossible to conduct further research on the mechanism of the carboxylic acid reduction reaction.

In your opinion, what are the key points when starting and in the early stages of the PhD path?

Certainly not a surprising answer, but networking is critical from the beginning. The scientific community is very open to cooperation, and I recommend planning internships in other units, joint projects and research from the beginning. Many grants support internships and promote projects that consider research in different units. Publications and subsequent projects always follow such activities, and after a PhD, this networking is vital for finding a post-doc position or writing your project.



Reconstruction of an AOR filament structure based on a structure from cryo-EM, mass photometry, and QM:MM calculations

Piotr Wróbel, PhD

Jagiellonian University in Krakow

The interview with the author of the PhD thesis:
"Studies of interactions in solutions based on Molecular Dynamics methods and simulated vibrational spectra"

What made you devote your doctoral thesis to interactions in solutions of selected substances with potential use in modern batteries?

When I started working with my team in 2017, my supervisor had already implemented a grant to research this topic. At that time, I carried out simulations for one such substance, and that formed the content of my master's thesis. The results were satisfactory and indicated the validity of the methodology applied to such systems. Hence, it was a natural decision to continue working in this field.

What was the most challenging aspect of your research regarding acquiring the data and developing the results based on it?

Regarding data acquisition, the biggest challenge was obtaining a meaningful learning set for training neural networks that predict potential energy for a given system geometry. This required careful selection of various geometries, including those with "unnaturally" stretched or bent bonds, so the learned model could predict that these were energy-disadvantageous structures.

In the case of developing the results, it was more like counting the residence time autocorrelation function due to the memory complexity of the algorithm used to calculate it and my – at the time – limited experience in implementing such issues.

Your dissertation presents potential alternatives to simulations using ab initio molecular dynamics (AIMD). How do you assess the need for solutions with lower computational costs?

I believe that developing methods with a lower computational cost and a sensible trade-off in the accuracy of the results compared to ab initio methods is desirable in the context of a more comprehensive application of such research in industry, for example. AIMD, despite leading to results close to experimental values, still requires relatively large computational time. For instance, it took about a month to obtain a 35 ps simulation for a system containing 50 molecules of ethylene carbonate (i.e., 500 atoms).

How did Cyfronet's resources benefit the part of your research related to calculations and their analysis?

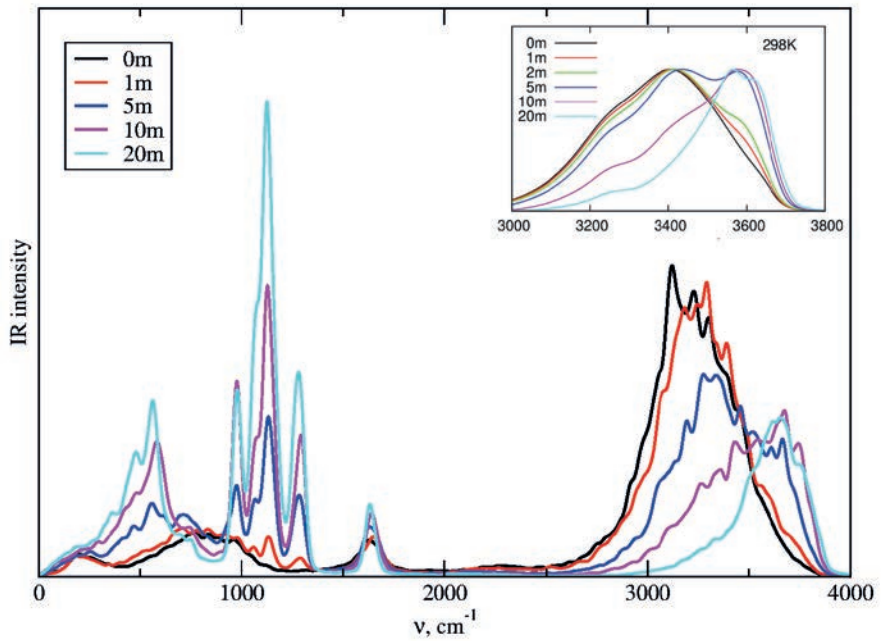
The resources of the Cyfronet made it possible to do any research – the Prometheus and then Ares supercomputers were used to run all simulations (AIMD or DFTB), and later, the dedicated Ares partition with GPUs was used to train neural networks.

What aspect of scientific work gives you the most satisfaction?

The most remarkable moment is the one of satisfaction, when, after a long period of work during which there was doubt, a clear and expected result finally begins to become apparent.

What could you advise individuals who are just beginning their doctoral studies? What should these individuals pay the most attention to?

I recommend finding the niche you like rather than looking at the activities of your teammates. And this is even though another team publishes more, has more grants, etc.; remember that the grass always seems greener on the other side of the fence. It is worth taking advantage of conference trips to get used to public speaking; after that, the thesis defense will no longer be a stress but a formality. In addition, it is essential to participate in research funding competitions. Even if the chances of winning are slim, the basic principle is simple – who does not apply wins nothing. Finally, unfortunately, there is also a very pragmatic note. If it is impossible to continue a scientific career after the doctorate, obtaining a qualification that allows for other professional work is invaluable. This provides a great deal of mental comfort.



Infrared spectra obtained from AIMD for LiTFSI in H_2O systems. The inset contains experimental spectra in the range of O-H vibrations from Y. Zhang, N. H. C. Lewis, et al., J. Phys. Chem. B 125 (2021), 4501–4513

Karolina Zawadzińska, PhD

Cracow University of Technology

The interview with the author of the PhD thesis:
"Synthesis of novel heterocyclic nitrocompounds via [3+2] cycloaddition reaction"

How could you briefly explain the subject of your research to a person unrelated to the field?

The subject of my research was the synthesis and theoretical description of biologically active cyclic organic compounds, which in their structure contain so-called heteroatoms – oxygen and nitrogen. In simpler terms, I studied the book course of reactions that I had previously managed to perform experimentally. In addition, in my work, I determined the potential biological activity of these compounds; that is, I determined their suitability for use as drugs or herbicides.

Your research used more than a dozen computational and experimental techniques, representing sequential steps to achieve your goals. To what extent was this sequence predetermined, and to what extent did you make flexible changes during the research?

In science, one must be flexible, but, of course, within reason. When describing chemical reactions theoretically, the course of calculations and the application of given calculation techniques are usually assumed in advance. Still, in practice, there are also deviations from the norm. As a scientist, when analysing the results obtained, I have to be flexible enough to base only on reliable results and not bend the theory just to fit into some assumptions. In science, sometimes we have to fit in with the object under study; it is rarely the case that it is the object that fits in with us. This is especially evident when experimenting in organic chemistry, where you often have to combine to "force" the object of study to cooperate.

What is the application potential of the obtained compounds?

The presence of heteroatoms in the structure of organic compounds increases their biological activity and, thus, the range of their potential applications. Many structurally similar compounds to those I synthesised are already used as anti-inflammatory drugs, but more importantly, as antiparasitic agents in veterinary medicine, such as Fluralaner used in the popular Bravecto agents for dogs and cats against ectoparasites. I decided to check these literature reports against my compounds. It turned out that a potential application of my isoxazolines is precisely for analgesics and anti-inflammatory agents.

What were the biggest obstacles in your research work, and how did you overcome them?

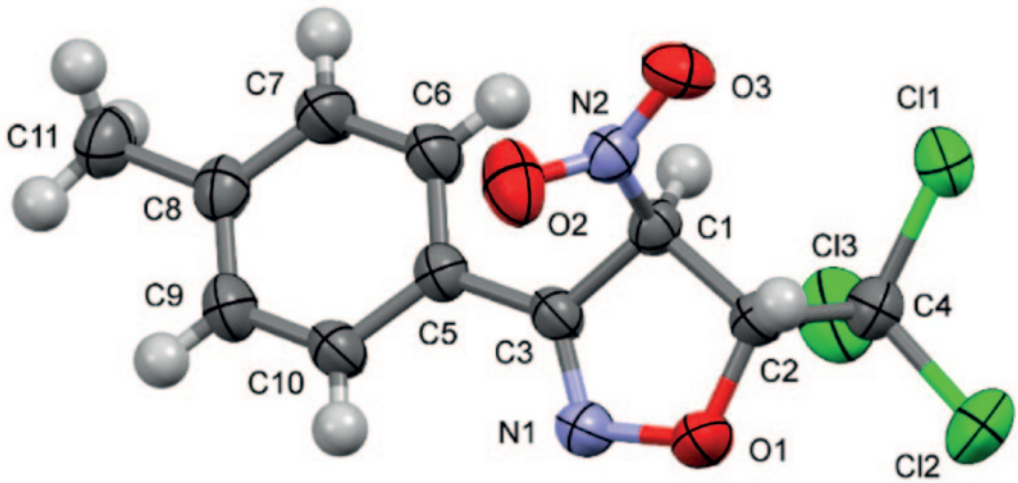
There were a lot of bumps and obstacles on the road to doing research for my dissertation. Every day brought new challenges, which were often hard to cope with. The most difficult, however, was the stage of synthesis and purification of the compounds I obtained. This stage required great dedication and patience, as well as teamwork.

How did Cyfronet's resources benefit the part of the research related to calculations and their analysis?

Without the possibility to use the computing power of Cyfronet's supercomputers, I would not have been able to carry out any research so efficiently. I based all my planned steps in my research work mainly on computer modeling of the course of the reaction to know whether it was feasible. Undoubtedly, the calculations helped reduce the time to find errors and experimental solutions; thanks to the calculations, I could save reagents, and finally, I could focus on those reactions that made some sense.

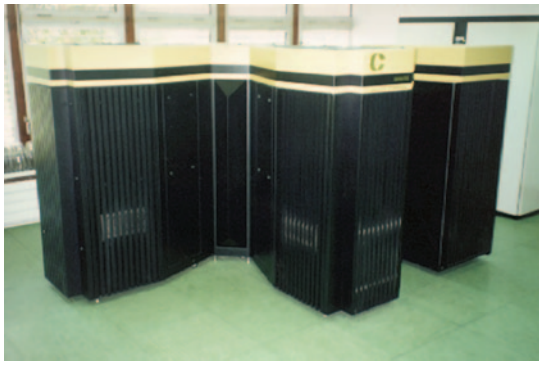
What advice or thoughts would you share with researchers just starting doctoral schools?

Do not give up! Conducting research in various fields, not only in chemistry, is very hard, and many of them may fail. However, remember that every result obtained is valuable! Be curious about all the details because sometimes they play a significant role. Be willing to go beyond the usual patterns.

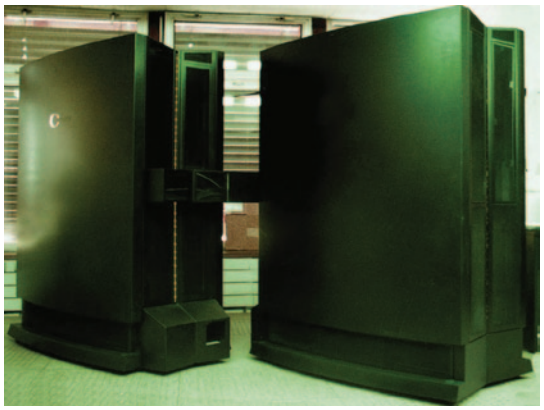


The molecular structure of isoxazoline, obtained from a crystal X-ray diffraction experiment

CDC CYBER 72



Convex C3840



Exemplar SPP1600/XA

1973 CYFRONET is established

1975 A CDC CYBER 72 computer is deployed at the Centre

1990 The first Kraków node of the EARN / BITNET network is deployed at CYFRONET (on an IBM 4381 computer)

1991 CYFRONET installs a Convex 120 machine – the first vector computer in Central and Eastern Europe.

The first Polish national Internet link is established between Kraków and Warsaw.

Construction begins in the Kraków MAN

1994 A 2 Mbps link is deployed between Kraków and Warsaw

1996 An Exemplar SPP1600/XA computer deployed at CYFRONET took a position on the TOP500 list.

The first automatic tape library (ATL 2640) is installed at the Centre

1997 The ATM communications subnet is deployed within the Kraków MAN.

CYFRONET joins the POL-34 national backbone

1998 An SGI Origin2000 computer is deployed at the Centre

2000 Increasing the Centre network connection bandwidth to 155 Mbps

2002 A RackSaver PC computer is deployed at CYFRONET as part of the CrossGrid project

2003 An HP Integrity SuperDome computer is deployed at CYFRONET (the first such computer in Poland)

2005 An HP Storage Works XP12000 disk array is deployed at CYFRONET.

Increasing the Centre network connection bandwidth to 622 Mbps

2006 An HP Storage Works EVA 8000 disk array and an SGI ALTIX 3700 supercomputer (Baribal), with 0.8 TFlops of theoretical peak performance, is deployed at CYFRONET

2007 An agreement concerning the creation of the Polish Grid (PLGrid) Consortium was signed.

An SGI ALTIX 4700 supercomputer with the SGI RASC acceleration module is deployed at CYFRONET.

IBM BladeCenter HS21 servers are deployed at CYFRONET (6.2 TFlops).

An HP Storage Works EVA 8100 disk array is deployed at CYFRONET

2008 The configuration of SGI ALTIX 3700 supercomputer is extended to 1.5 TFlops.

MAN 10 Gbps started.

The Metropolitan Area Network is directly connected to Warsaw and Bielsko-Biała through the PIONIER network links, each of 2x10 Gbps capacity.

Zeus supercomputer (HP Cluster Platform 3000 BL) with 2 048 cores is deployed at CYFRONET

2009 Start of the PL-Grid project – Polish Infrastructure of Supporting Computational Science in the European Research Space

2010 The configuration of Zeus supercomputer is extended to 9,544 Intel Xeon cores, Zeus has been placed on 161st position on the TOP500 list

2011 Deployment of Hitachi Data Systems High Performance NAS Platform for computing infrastructure.

Total amount of installed disk space exceeds 2 PB.

The configuration of Zeus supercomputer is extended to 12,032 Intel Xeon cores.

Zeus has been placed on 80th position on the TOP500 list

2012 Start of the PLGrid Plus project – domain-oriented services and resources in the PL-Grid.

In April, ScaleMP, a leading provider of virtualisation solutions for high-end computing, announced that Zeus-vSMP system at CYFRONET is the largest virtual SMP system in Europe.

Zeus among 100 fastest supercomputers on the TOP500 list.

The Metropolitan Area Network is directly connected to Rzeszów through the PIONIER network link of 2x10 Gbps capacity

SGI Origin2000

SGI ALTIX 3700

HP Cluster Platform 3000 BL

Anniversary Medal

New Machine Hall

Prometheus supercomputer

2013 After upgrading of Zeus supercomputer configuration to 25,468 cores, its theoretical peak performance reached 374 TFlops.

Anniversary Medal has been minted

2014 The new Machine Hall is completed.

Start of two new projects – PLGrid NG and PLGrid Core.

The Metropolitan Area Network is directly connected to Katowice through the PIONIER network link of 2x10 Gbps capacity

2015 The Prometheus supercomputer (41,472 cores) is deployed at CYFRONET, and ranks high, 49th place on the TOP500 list (the July edition), and next (after upgrading to 53,568 cores) 38th place (the November edition).

For the first time in history two supercomputers from Cyfronet (Prometheus and Zeus) are ranked on the TOP500 list, in one edition.

The new backup Data Center is completed.

CYFRONET starts active participation in INDIGO-DataCloud, EGI-Engage, EPOS-IP and PRACE-4IP projects.

High Performance Computing centres in Poland (Gdańsk, Kraków, Poznań, Warsaw and Wrocław) are integrated with links of 2x100 Gbps capacity

2016 Prometheus ranks 48th (the June edition) and 59th place (the November edition) on the TOP500 list

2017 Prometheus ranks 71st (the June edition) and 77th place (the November edition) on the TOP500 list.

Further dynamic development of the Centre, including establishment of 6 new laboratories.

Sat4Envi, Gliomed, EPOS-PL and eXtreme DataCloud projects launched

2018 Prometheus (53,604 cores, 2.4 PFlops) ranks 103rd place (the June edition) and 131st (the November edition) on the TOP500 list.

EOSC-Hub and PRIMAGE projects have been launched

2019 Cyfronet represents Poland in the LUMI consortium, composed of eight countries that will jointly build one of the fastest European supercomputers.

Prometheus ranks 174th place (the June edition) and 241st place (the November edition) on the TOP500 list.

Cyfronet exhibition stand at the ISC'19 conference.

Cyfronet provides a new computational system for research using AI methods, with computational power over 4 PFlops for tensor operations and 256 TFlops for standard calculations.

PRACE-LAB, PRACE-6IP, SANO, EOSC-Synergy and EOSC Enhance projects launched

2020 Among the strategic infrastructures included in January 2020 on the Polish Research Infrastructure Map there are two projects proposed by ACC Cyfronet AGH as the initiator and coordinator of the PLGrid consortium: *National Supercomputing Infrastructure for EuroHPC* and *National Cloud Infrastructure PLGrid for EOSC*.

Prometheus (53,748 cores, 2.7 PFlops) ranks 288th place (the June edition) and 324th (the November edition) on the TOP500 list.

The Prometheus supercomputer supports scientists in the fight against coronavirus.

EPOS PL +, PRACE-LAB2, EPOS SP, PROTEUS-RS and EUROCC projects launched

2021 The Ares supercomputer with theoretical peak performance over 4.0 PFlops is deployed in Cyfronet.

Prometheus ranks 373th and 440th place, and Ares ranks 216th and 267th place on the TOP500 list.

A new version of the ACC Cyfronet AGH website has been launched.

EuroHPC PL, PIONIER-LAB, KMD3, AGH – PANDA3, EGI ACE, EOSC Future and FINDR projects launched

2022 Athena supercomputer with theoretical peak performance 7.7 PFlops is deployed in Cyfronet.

Opening of the Data Center Podole.

For the first time in the history of Polish computer science, three supercomputers from one Polish computing centre (Athena, Ares and Prometheus) are ranked on the TOP500 list.

Prometheus (53,748 cores, 2.7 PFlops) ranks 475th place, Ares (37,824 cores, 4 PFlops) ranks 290th and 323rd place and Athena (6,144 cores, 7.7 PFlops) ranks 105th and 113th place on the TOP500 list.

Inauguration of the LUMI supercomputer.

EUMaster4HPC, FAIRCORE4EOSC, EuroScienceGateway, InterTwin, DT-GEO, Geo-INQUIRE and EDITH projects launched

2023 Celebration of the 50th anniversary of Cyfronet AGH with the participation of President Andrzej Duda, who presented state decorations to distinguished employees of Cyfronet.

Athena ranks 123rd place and Ares ranks 362nd place on the TOP500 list.

Cyfronet AGH honored with the Polonia Minor Award.

The EuroHPC PL project team was the winner of the Polish Smart Development Award 2023.

For the second time in the history of Polish computer science, three supercomputers from one Polish computing centre (Athena, Helios CPU and Ares) are ranked on the TOP500 list (the November edition) in places 154th, 290th and 403rd respectively.

DOME, EUROCC 2, EUreka3D, PIONIER-Q and GEMINI projects launched

2024 For the first time in the history of Polish computer science, four supercomputers from one Polish computing centre (Helios GPU, Athena, Helios CPU and Ares) are ranked on the TOP500 list (the June edition) in places 55th, 177th, 305th and 442nd, respectively.

Helios GPU ranked 3rd place on the Green500 list (the June edition).

Four supercomputers from Cyfronet (Helios GPU, Athena, Helios CPU and Ares) are again ranked on the TOP500 list (the November edition) in places 69th, 212th, 348th and 490th, respectively.

Meetween, EOSC Beyond, EPICURE, FFplus, PLGrid ICON and EPOS ON projects launched

AGH UST Campus

LEGEND

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4. Faculty of Electrical Engineering, Automatics, Computer Science and Biomedical Engineering
5. Faculty of Computer Science, Electronics and Telecommunications
6. Faculty of Mechanical Engineering and Robotics
7. Faculty of Geology, Geophysics and Environmental Protection
8. Faculty of Mining Surveying and Environmental Engineering
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