
Delivering enhanced supercomputing performance for Vilnius University



Vilnius
universitetas

Atos

Unprecedented opportunities for Lithuania's academic, research and business communities

Atos helps Vilnius University to increase the productivity of its supercomputers by more than ten times



Outcome statistics/metrics

- Estimated total system performance at least 0.5 petaflops, with total RAM more than 50 terabytes per task
- Use of up to 0.3 petaflops performance computing power for a single task
- Over 0.2 petaflops GPU subsystem performance

“World-class experimental, technological research and fundamental theoretical modeling work are carried out at the Faculty of Physics of Vilnius University. The supercomputer part and software of the Faculty of Physics are adapted to this work, which requires the largest possible number of processors and very large RAM. In addition to our own research, and collaborations with CERN and with other universities, it is gratifying that there are small high-tech companies that also need supercomputer resources and will be able to take advantage of the services provided by the EuroHPC Center of Excellence.”

Professor Juozas Šulskus
Dean, Faculty of Physics,
University of Vilnius

Executive summary

With VU HPC, the largest supercomputer in Lithuania, Vilnius University can leverage more from machine learning, artificial intelligence and big data. Innovations are creating new opportunities for science and research, and competitive edge for business and the economy. While VU HPC resources are also distributed in the University's Faculty of Mathematics and Informatics, this case study focuses on the Faculty of Physics.

1 Challenge: Advancing ground-breaking research

Requirements at the Vilnius University and University's Faculty of Physics have grown significantly, particularly in relation to machine learning, quantum computing and data analytics. With the importance of multi-disciplinary research and ever-increasing volumes of analyzed data, the Faculty needs extremely high-performance computing (HPC) power and graphical computing processors.

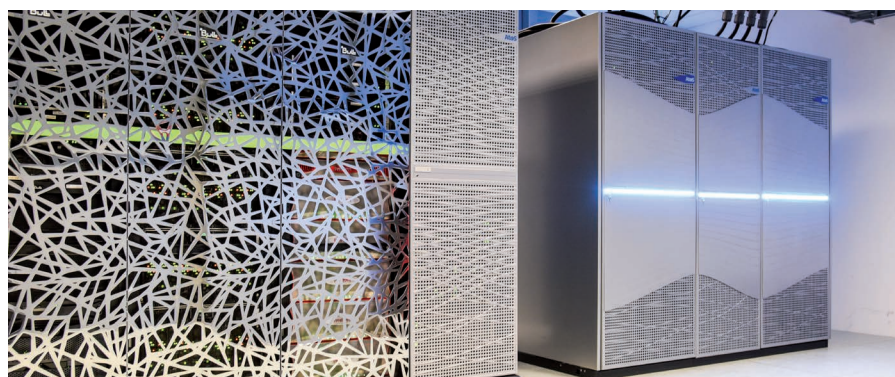
2 Solution: New powerful supercomputing resources

Working in partnership, UAB Bull Baltija (an Atos company) together with Atos partner Duvait UAB (who has over 15 years' experience in HPC, networking, security and data center solutions) integrated and installed new hardware, software and storage facilities in an HPC cluster with more than 4,500 computing cores and almost 55TB of RAM.

The Faculty of Physics planned that the HPC solution be located in the newly built National Center of Physical and Technology Sciences. This required relocation of the current HPC solution to a new location, expansion of cooling and power capabilities of data center and integration of all components was completed by Atos partner - Duvait UAB. This partner also performed an implementation of the new Atos BullSequana supercomputer and delivery of required Direct Liquid Colling (DLC) system and will provide 24x7 maintenance services for the whole solution. As a result, all Faculty of Physics HPC resources are managed from a single-pane-of-glass management system and can leverage various tasks for research. In the scope of the same project, the high-speed and high-availability network infrastructure was implemented for other Faculties and EuroHPC data connection.

The Atos BullSequana supercomputer, incorporating the latest processor and accelerator architectures, provides increased high-quality multidimensional computing power. With the help of artificial intelligence, it expands the possibilities of HPC modeling and helps users to go beyond traditional modeling.

One of the supercomputing facility's key features is the broad range of tasks and users it supports - from researchers requiring extremely large computing resources to IT specialists or students looking for flexible computing capabilities. Its infrastructure operates on the principles of open access and is accessible not only to members of the University community but also to Lithuanian companies, start-ups and state institutions, contributing to the competitiveness of Lithuania and its research and academic community.



Example applications

VU HPC will be used for the modeling of electronic systems of light energy capture and photosynthetic molecular electronics materials by quantum chemical methods. The main and excited states of PI electronic systems - carotenoids, photosynthetic compounds based on them, with allowable and forbidden electronic states - will be analyzed. Raman spectra of these compounds, dynamic characteristics of excited states, the possibility of proton transfer in conjugated systems, and graphene layers will be modeled. Organic materials and devices are expected to be widely used in fields ranging from medicine to energy and computing. For this purpose, optically active molecular aggregates are widely studied. Methods for modeling quadrupole nuclear magnetic resonance relaxation parameters will be developed. The developed methods will be implemented in a computer system that will be applied in the theoretical research of biomolecular systems and nanostructured properties. It is planned to develop the work of characterization of new molecular devices from structural and energy parameters. Small-sized nanostructures (pi-conjugated structures with multiple penta-sixta-ring substituents) are promising for molecular structure and single-controlled processes on nano-micrometric distance scales, as well as for the formation of self-assembled surface coatings with ordered or controlled properties. With a much more powerful HPC system, VU researchers have the opportunity to model for quantum computers based on molecular compounds and to develop algorithms for quantum calculations.

In addition to Vilnius University (VU) research projects, CERN and VU cooperation projects, development works of parallel algorithms developed by Vilnius Gediminas Technical University researchers, and projects of Vytautas Magnus University biochemists are carried out using a supercomputer. Also undertaken are economists' statistical econometric modeling works and astrophysical modeling works of stellar atmospheres and observed star properties.



3 Benefits delivered: The University of Vilnius is helping to advance Lithuania's research, academic and business community on the world stage

- Based on its new resources, Lithuania's plans include membership of EGI (European Supercomputer Network), allocating up to 30% of efficient computing resources to EGI infrastructure as needed.
- On the basis of the new supercomputer, Lithuania became a member of the European project EuroHPC, and Vilnius University is Lithuania's representative in the joint EuroHPC Center for Competence in Efficient Computing to provide supercomputing capabilities, not only to scientists, doctoral students and researchers, but also to high-tech medium and small businesses.
- With the introduction of the new EuroHPC supercomputer systems, Europe will become an equal partner to the United States and China in terms of computing resources; Lithuanian researchers can use the common European resources for the development of quantum computer technologies at close to 1 exascale.

4 Why Atos? Boost your power to innovate

Atos is Europe's largest supercomputer manufacturer. Our BullSequana X series of servers provides maximum flexibility in terms of interconnect, power and cooling, and covers the widest-possible spectrum of applications. BullSequana X supercomputers offer an infinitely adaptable response, with a large choice of compute nodes, accelerated nodes and specialized nodes. And this multitude of components can be combined, in a completely customized way, into a single system and managed as a single system using the Bull supercomputer suite.

About Vilnius University

Since its establishment in the 16th century, Vilnius University, as integral part of European science and culture has embodied the concept of a classical university and the unity of studies and research.

Vilnius University is an active participant in international scientific and academic activities and boasts many prominent scientists, professors and graduates. Scientific development and the expanding relations with global research centres have contributed to the variety of research and studies at Vilnius University.

With the support of social partners, the university educates globally-minded specialists who successfully integrate in the modern European community.

Writing your
story with
your business
technologists

About Atos

Atos is a global leader in digital transformation with 110,000 employees and annual revenue of € 12 billion. European number one in cybersecurity, cloud and high performance computing, the group provides tailored end-to-end solutions for all industries in 73 countries. A pioneer in decarbonization services and products, Atos is committed to a secure and decarbonized digital for its clients. Atos operates under the brands Atos and Atos|Syntel. Atos is a SE (Societas Europaea), listed on the CAC40 Paris stock index.

The purpose of Atos is to help design the future of the information space. Its expertise and services support the development of knowledge, education and research in a multicultural approach and contribute to the development of scientific and technological excellence. Across the world, the group enables its customers and employees, and members of societies at large to live, work and develop sustainably, in a safe and secure information space.

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Let's start a discussion together

