IT4Innovations Supercomputers will help find a cure for coronavirus

Ostrava, 18th June 2020 – High-performance computers in the Czech Republic are again serving a good cause. IT4Innovations National Supercomputing Center has started cooperation with the Italian university Politecnico di Milano and offered a hand in the research connected with the most discussed disease of this time – COVID-19.

In recent months, coronavirus has paralyzed the economy of many countries, has caused the collapse of many of health institutions and left hundreds of thousands of deaths behind. A number of scientists are now focused on searching for medication that would cure people infected with the disease COVID-19. However, the process of discovering new medication is very expensive and the medication reaches the market after many years of testing. This problem can be helped by supercomputers which manage to boost the testing significantly and thus reduce the investment. Considering this fact, especially pharmaceutical companies are starting to invest in supercomputing resources and cloud solutions, because high-performance computing resources, new numerical models and artificial intelligence enable the creation of simulations with more precise computing in a significantly shorter time.

In the past IT4Innovations National Supercomputing Center cooperated with Politecnico di Milano on the project ANTAREX. A case study of the ANTAREX project, in collaboration with Dompè Pharmaceutical and CINECA supercomputing center, gave birth to a platform for drug discovery (called Exscalate) against pandemic viruses and other pathogens. This platform was tested later also in connection with the Zika virus. Nowadays, the above mentioned platform is used within the project Exscalate4COV in order to find medication against coronavirus. The number of chemical substances that could contribute to the cure of the disease COVID-19 has risen from 1 billion to 500 billion, which makes the whole analysis very demanding. Scientists from Politecnico di Milano are planning to optimize the above mentioned platform also with the utilization of Czech supercomputers located in IT4Innovations in Ostrava and to simplify the remote execution of computation on supercomputers by means of HPC-as-a-Service solutions HEAppE developed in IT4Innovations. Another aim of the cooperation is to find out if there is a possibility to use artificial intelligence to determine particular substances which would be preferentially analyzed in future extreme situations.

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

"*Within the project Exscalate4COV, an initial investigation on the reduced database of 10, 000 available drugs has been already done, and currently the challenging part is to extend it to more than 500 billion molecules. Here is where supercomputers make the difference by supporting a fast selection of only the most promising molecules to be sent to the subsequent phases of the drug discovery pipeline. The experience we had in the ANTAREX project with IT4Innovations was successful and the current*

collaboration can help us in further accelerating the computational process for facing a future pandemic," said Gianluca Palermo, Politecnico di Milano principal scientist in the Exscalate4COV project.

Media contact

Zuzana Cervenkova, Spokesperson for IT4Innovations National Supercomputing Center

zuzana.cervenkova@vsb.cz

Phone: +420 602 593 335

IT4Innovations National Supercomputing Center provides Czech and foreign research teams, from both academia and industry, with state-of-the-art HPC and data analysis technologies and services. IT4Innovations currently operates four supercomputers – Anselm (launched in summer of 2013, 94 TFlop/s), Salomon (launched in summer of 2015, 2 PFlop/s), Barbora (launched in autumn of 2019, 849 TFlop/s), and NVIDIA DGX-2, a specialized system for artificial intelligence calculations, (launched in spring of 2019, 130 TFlop/s ando 2 PFlop/s in AI). In 2021, a petascale system entitled EURO_IT4I is to be launched within the EuroHPC project. IT4Innovations is also a research centre with strong international links. The key research areas of IT4Innovations include big data processing and analysis, machine learning, development of parallel scalable algorithms, supercomputing technology development, solution of computationally demanding engineering problems, advanced visualization, virtual reality, modelling for nanotechnologies and material design. IT4Innovations is part of VSB – Technical University of Ostrava. For more information, see www.it4i.cz.

Politecnico di Milano is a scientific technological university which trains engineers, architects and industrial designers. The University has always focused on the quality and innovation of its teaching and research, developing a fruitful relationship with business and productive world by means of experimental research and technological transfer. Research has always been linked to didactics and it is a priority commitment which has allowed Politecnico Milano to achieve high quality results at an international level as to join the university to the business world. Research constitutes a parallel path to that formed by cooperation and alliances with the industrial system. For more visit www.polimi.it/en