PRESS ANNOUNCEMENT

LIGATE: NEW EUROPEAN BACKED EFFORT AGAINST PANDEMICS KICKS OFF WITH 5,9 MLN €

- **LIGATE will develop the leader software application for Drug Discovery exploiting today's high-end supercomputer and tomorrow's Exascale-acquired resources.**

- **The portable and tunable drug discovery platform will allow a drug discovery campaign in less than one day to respond promptly to worldwide pandemic such as that due to coronavirus.**

- **Following the successful results and data generated by EXSCALATE4COV[1] project, which identified some antiviral molecules and is testing one (raloxifene) in phase II/III clinical trials, LIGATE plans to publicly disclose to the scientific community also the result of a large experiment against immune resistant targets.**

- **LIGATE will run for a 3-year period with a total funding of €5.9 million, co-funded by European High-Performance Computing Joint Undertaking[2] (JU) with €2.6 million.**

Milano, 16.02.2021 - Italy is leading LIGATE, the public-private consortium funded by the EU and the JU's member Countries for projects innovating and widening the use of High Performing Computing (HPC).

The consortium, coordinated by Dompé Farmaceutici, was awarded by the European Commission with the primary objective to exploit the potential of supercomputing

[1] www.exscalate4cov.eu

[2] https://eurohpc-ju.europa.eu

combined with life science scientific skills in Europe to better and quickly face pandemic situations of supranational interest.

The consortium aggregates 11 institutions and companies in five European countries including Politecnico di Milano (Department of Electronics, Information and Bioengineering), CINECA Interuniversity Consortium (Supercomputing Innovation and Applications), E4 Computer Engineering, University of Salerno, University of Basel, KTH Royal Institute of Technology (Department of Applied Physics), University of Innsbruck, tofmotion GmbH, IT4Innovations National Supercomputing Center, and Chelonia Applied Science.

The LIGATE project will enable the Dompé Farmaceutici EXSCALATE platform to exceed the existing performance, namely the ability to evaluate 1 trillion molecules per simulation, by enhancing the quality of the simulations with a deeper integration of Artificial Intelligence and Machine learning and at the same time by further accelerating their throughput.

Fostering the European competitiveness in the field, EXSCALATE solution is an indispensable tool in the long process of drug discovery and development. It also provides options for understanding chemical systems in different ways, yielding information that is not easy to obtain in laboratory analysis, with considerably less cost and effort than experiments.

The multidimensional workflow of the project is distributed among the participants as follows.

POLIMI will develop open-source tools to support the optimization and tuning of parallel applications, and in particular the EXSCALATE platform, on novel heterogeneous architectures. Moreover, POLIMI will drive the development of the molecular docking procedure with the integration of Machine Learning techniques always keeping in mind the urgent computing scenario

In accordance with its institutional mission, CINECA plays the role of a high technology bridge between the academic and research world and the industry and public administration world. The main goal of CINECA in LIGATE is to validate and deploy the CADD solution on its systems, including the EuroHPC pre-exascale Leonardo system, and making it available to the academic and industrial users.

EXSCALATE will be ported on various modern heterogeneous accelerator clusters based on the CELERITY[3] platform which is built on top of Khronos' emerging industry standard SYCL 2020 for accelerator programming and which will be released as open source by project partners University of Innsbruck and University of Salerno. CELERITY will be extended as part of LIGATE to substantially simplify code development, porting, scaling and optimization for performance and energy targeting CPU/GPU/Tensor platforms.

[3] https://celerity.github.io/

In LIGATE, The University of Basel will benchmark the structure-based drug discovery solutions developed within LIGATE using established community data sets and validate them on relevant real-world use cases.

tofmotion will be provided with a much faster and more accurate simulation of Time-to-Flight 3D-cameras based on LIGATE technologies.

KTH will consider development of modules building on the open source tools to provide fully automated efficient free energy calculation that includes both parametrization of compounds, set-up and automated execution of all required simulations. This could be exploited in combination with commercial support activities, although we anticipate all software to be available without charge to the academic research community.

IT4Innovations will provide the software improvements in HyperLoom software stack for the LIGATE project; all updates and improvements will be open sourced and utilised in other projects related to scientific pipelines. Besides that, IT4Innovations will also validate and exploit the LIGATE solution on its systems, including the EuroHPC petascale system Karolina.

Within the project, E4 Computer Engineering SpA will provide remote access to a number of heterogeneous hardware CPU/GPU/Tensor platforms to enable the developers of the structure-based drug discovery tools to test the open source tools on advanced plug-and-play platforms.

Dissemination of results and exploitation activities are provided by the Swiss CHELONIA APPLIED SCIENCE.

The partners will constantly upload the contents on the website www.ligateproject.eu.