PRESS RELEASE

Exscalate4CoV[1] can now count on the two most powerful supercomputers in Europe in the race against the coronavirus

30 June 2020 - Exscalate4CoV, the private-public consortium supported by the EU's Horizon 2020 programme for research and innovation, led by Dompé Farmaceutici and currently representing 18 partners, during past months has intensively used the competences and the resources of the European supercomputing centers installed at Eni, CINECA, Barcelona Supercomputing Center and FZ Juelich to simulate the interactions between the proteins of the coronavirus SARS-CoV-2 and the molecules of potential therapeutic drugs, in a race against time to identify a therapy to fight the virus effectively.

The activities of the **Exscalate4COV** Task Force on High Performance Computing coordinated by the partner Politecnico di Milano can now count on **the two most powerful supercomputers in Europe.** According to the TOP500 list of the fastest supercomputers in the world, announced on June 22, 2020 at the ICS High Performance virtual conference, these two supercomputers are installed in Italy: the new **HPC5** system at the energy company Eni and the **Marconi-100** system at the CINECA Italian supercomputing center.

The number one in Europe (number six in the TOP10 list worldwide) is the new **HPC5 system** installed at Eni reaching 35.5 PetaFLOPS (million billion operations per second) and 51.7 PetaFLOPS peak performance. HPC5 is a PowerEdge system built by Dell and powered by Intel Xeon Gold processors, NVIDIA Tesla V100 GPUs and Mellanox HDR InfiniBand network. The second fastest supercomputer in Europe is **Marconi-100,** powered by IBM Power9 processors, NVIDIA V100 GPUs and dual-rail Mellanox EDR InfiniBand network. Marconi-100 reached 21.6 PetaFLOPS and 29.4 PetaFLOPS peak performance and became the number nine on the TOP10 list worldwide.

[1] The **Exscalate4CoV (E4C) (www.exscalate4cov.eu)** private-public Consortium is coordinated by Dompé Farmaceutici, and is comprised of eighteen institutions and research centers from seven countries around Europe: Politecnico di Milano (DEIB), CINECA (Supercomputing Innovation and Applications), Università degli Studi di Milano, Katholieke Universiteit Leuven, International Institute of Molecular and Cell Biology in Warsaw (IIMCB), Elettra-Sincrotrone Trieste, Fraunhofer Institute for Molecular Biology and Applied Ecology, Barcelona Supercomputing Center, Forschungszentrum Jülich, Università Federico II di Napoli, Università degli Studi di Cagliari, SIB Swiss Institute of Bioinformatics, KTH Royal Institute of Technology, Associazione Big Data, Istituto Nazionale di Fisica Nucleare (INFN), Istituto Nazionale per le Malattie Infettive Lazzaro Spallanzani and Chelonia Applied Science.

Thanks to the recent investments planned in Europe, new further systems are underway: **Leonardo** supercomputer, which will be hosted at Bologna Science Park Italy, and the **MareNostrum 5** supercomputer, which will be placed in Barcelona Supercomputing Center, Spain. Those systems, procured by EuroHPC Joint Undertaking initiative and 50% co-funded by the hosting participating States, will have by design a sustained performance to be ranked among the five most powerful supercomputers in the world.

Currently, Exscalate4COV's supercomputers are already processing chemical data at high speed. With the availability of Eni's HPC5 and Marconi-100 systems, the Exscalate4COV will push further to win the race against time, and against the virus. At the core of the project is **Exscalate** (EXaSCale smArt pLatform Against paThogEns), at present the most powerful (and cost-efficient) intelligent supercomputing platform in the world. Exscalate platform leverages a "chemical library" of 500 billion molecules and represents a powerful tool to accelerate the "in-silico" computational phase of development of new therapies, called virtual screening process, which needs to exploit at the best the underlying supercomputing resources. To reach its objectives, Exscalate4COV Consortium can leverage not only on the most powerful supercomputers in Europe, but also on some of the best computational and life-science research labs in Europe to counter international pandemics faster and more efficiently.

During the last months, the first virtual (in silico) screening phase was run on the Consortium's supercomputers to process more than 400.000 molecules (safe-in-man drugs and natural products) made available by Dompé Farmaceutici and the partner Fraunhofer (IME). Overall 7.000 molecules with certain promising characteristics were tested. Priority in testing was given to molecules in clinical stage or already on the market. As a main outcome of this first "in-silico" project phase, Exscalate4Cov recently announced that **Raloxifene** was effective against SARS-Cov-2 in-vitro, countering the replication of the virus in cells. The IP for its use against Sars-Cov2 has already been protected on behalf of consortia members. Dompé has requested access to clinical trials to establish the efficacy of Raloxifene in Covid-19 patients.

In the second phase of virtual screening, the Exscalate platform will exploit **HPC5** and **Marconi-100,** the two most powerful supercomputers in Europe to find highly specific new molecules for the development of post-emergency solutions for SARS-CoV-2. During this second phase, the virtual screening will then be extended to the overall chemical library of 500 billion molecules, thanks to the Exscalate processing capacity of more than 3 million molecules per second. The most promising interactions will then be studied and validated in the subsequent phases of the drug discovery pipeline. This enormous effort will receive experimental validation by the capabilities of the Consortium partners, both in the direction of structural complexes elucidation and in the direction of mechanistic elucidation at biochemical and cellular levels.

Links:

TOP500 List, June 2020: https://www.top500.org/lists/top500/2020/06/

Coronavirus: Using European supercomputing, EU-funded research project announces promising results for potential treatment, **European Commission official website -** 06/18/2020
https://ec.europa.eu/commission/presscorner/detail/en/ip_20_890