A supercomputing platform for Europe: Empowering smart in-silico drug design for addressing the COVID-19 virus

Call for collaboration with European pharmaceutical industries

Exscalate4CoV is an EU-funded project that was selected after the emergency Call of expression of interest that the European Commission (DG RTD) issued on 31 January. The project will receive a 3 million EUR of EU funding in the next 18 months. It is consisting of a coalition of three of the most powerful supercomputing centres in the EU (CINECA in Italy, Barcelona supercomputing center and Julich supercomputing center in Germany) together with a pharmaceutical company and several big Institutes dealing with biology and bio-molecular dynamics. They use supercomputers in the search of a therapy (drug) against COVID19 by complementing the classical trial and error clinical approach and possible experimentation in patients, by comparing the signature of the protein of the virus against active molecules that are used in existing databases of compounds.

The project is currently processing digital models of the protein of the virus and is matching them against a publicly available database of thousands of known active anti-molecules that are part of existing drugs with the aim to find out which combinations of active molecules could react to the virus. Very first promising outcomes of this matching operation (docking) are now becoming available. A large number of biologists and biochemists (both from the project as well as from many other institutes that have been associated to the aims of the project) are now proceeding to the biological screening of the identified promising molecules (lab experimentation) with the aim to come up with first results of a possible drug.

It comes out that the available computing power is sufficient for the docking operations. A key success point is the number of active anti-molecules that are part of existing drugs to which the project has access and is using for its docking operations.

We call the pharmaceutical companies and biochemical institutes of Europe that possess such databases of active molecules to make them available to the project (for example, via dedicated non-disclosure agreements). This would help the project enlarge its docking operations in the rapid search of a cure against COVID19.