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European researchers conduct 'biggest ever' COVID supercomputer test

By Reuters Staff

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MILAN (Reuters) - A European research consortium said on Monday it had carried out the most complex supercomputing experiment ever conducted on the new coronavirus, during a 60-hour simulation aimed at modelling the effect of potential new COVID drugs.

The operation, overseen by the European Commission-backed Excalate4Cov platform, harnessed supercomputers of Italy's Cineca computing consortium and energy giant ENI, testing 70 billion molecules and evaluating 1 trillion interactions.

"We reached the new goal of 5 million simulated molecules per second. As a comparison, ours is more than 300 times bigger and 500 times faster than the one carried out in the U.S. last June," said Andrea Beccari, head scientist of the project.

As drugs makers have raced to develop vaccines for COVID-19, researchers have turned to advanced supercomputers to crunch enormous quantities of data on a virus that was unknown a year ago and which has taken more than 1.3 million lives since it emerged in December.

The Excalate4Cov platform led by Italy's Dompé Farmaceutici is backed by the European Commission and coordinates supercomputing centres in Italy, Germany and Spain with pharmaceutical companies and research centres, including the University of Louvain, Fraunhofer Institut, Politecnico di Milano and Spallanzani Hospital.

The operation last weekend was carried out on computers operating at 81 Petaflops (one Petaflop is a unit of computing speed equal to one thousand trillion operations a second).

A first phase of the project ended with the identification of a generic osteoporosis drug that researchers hope may also help reduce COVID-19 symptoms, which last month got the go-ahead for human clinical trials by Italy's main medicines regulator.

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