

Lessons learned from urgent computing in Europe: tackling the COVID-19 pandemic

A team of authors from the PRACE Scientific Steering Committee, the PRACE Access Committee, and the PRACE Governance, and directors of European supercomputing centres, summarised the lessons learned from the 'PRACE Fast Track Call for Proposals to mitigate the impact of the COVID-19 pandemic' in a paper entitled 'Lessons learned from urgent computing in Europe: Tackling the COVID-19 pandemic'. This summary, including recommendations for future initiatives was published as published online at: www.pnas.org with DOI number 10.1073/pnas.2024891118.

The paper analyses various scientific efforts undertaken in Europe to combat the COVID-19 pandemic based on advanced and computationally intensive numerical simulations that require the use of large-scale computers. The five largest European supercomputing centres supported some of these efforts with free-of-charge computational resources, through the Partnership for Advanced Computing in Europe (PRACE).

The paper presents a number of computational models and methods relevant to the fight against the COVID-19 pandemic, including bio-structural studies, docking and screening for pharmaceutical applications, computational fluid dynamics to study droplet spread and transmission of the virus, organ modelling to support diagnosis and treatment of the disease, and epidemiology. We discuss the use of artificial intelligence (AI) in these areas and the readiness of the codes to run on high-performance computers.

"As an international association, we are proud of this publication, as both the activities from which the content of the paper is drawn, as well as the creation of the paper itself, show the high level of cross-border and cross-disciplinary collaboration and exchange that we are continuously striving for," said Serge Bogaerts, Managing Director of PRACE aisbl.

To find the full paper go here <https://www.pnas.org/content/118/46/e2024891118> or download the PDF at the end of this announcement.

About PRACE

The Partnership for Advanced Computing in Europe (PRACE) is an international non-profit association with its seat in Brussels. The PRACE Research Infrastructure provides a persistent world-class High-Performance Computing service for scientists and researchers from academia and industry in Europe. The computer systems and their operations accessible through PRACE are provided by five PRACE members (BSC representing Spain, CINECA representing Italy, ETH Zurich/CSCS representing Switzerland, GCS representing Germany and GENCI representing France). The Implementation Phase of PRACE receives funding from the EU's Horizon 2020 Research and Innovation Programme (2014-2020) under grant agreement 823767. For more information, see www.prace-ri.eu

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