Viral lessons from supercomputing

November 1 2021

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Swift, effective action is essential to face any crisis decisively. And, if it's a global one like the COVID-19 pandemic, these actions need to be efficiently coordinated to increase their impact while lessening the initial threat. This is exactly what the PRACE COVID-19 Fast Track Call set out to achieve, by allocating thousands of years of computer simulations (free of charge) to help fight COVID-19. Now, the scientific community is reaping the lessons that stemmed from the initiative.

The research carried out through the COVID-19 Fast Track Call has

brought in some interesting lessons for the scientific community. Prof. Núria López, ICIQ group leader and member of the PRACE Scientific Steering Committee (SSC), is the first author of the paper "Lessons learned from urgent computing in Europe: Tackling the COVID-19 pandemic" just published in the journal *Proceedings of the National Academy of Sciences* (*PNAS*).

When the COVID-19 pandemic hit Europe in early 2020, PRACE put into practice a long-planned idea of a fast-track program for crises situations: the COVID-19 Fast Track Call. The idea behind the Call is that simulations are often the first, essential step in a chain of value that, for example, leads in its very last phase to the approval of new medicine. Therefore, the allocation of free-of-charge High Performance Computing (HPC) resources—as well as ensuring the availability of the results to the whole community through the Open Science principles—would accelerate the generation of sound scientific knowledge. This would, in turn, catalyse and focus research in a particular area, creating hotspots of scientific activity.

"We saw there was a need as well as an opportunity to do urgent computing, and now we have our tools ready to face these kinds of challenges. This experience has taught us a lot and, when a new crisis arises, we'll be able to do it again. Open Science is particularly important in times of need," explains Prof. López.

In four months, the COVID-19 Fast Track Call received 80 proposals, showing the commitment of the scientific community to help in times of need. The incoming project proposals were divided into five broad groups: biomolecular research, screening of compounds, fluid dynamics, virus transmission via droplets, and epidemiology. Furthermore, twelve of the projects also used Artificial Intelligence (AI) techniques to model the spread of infections or do bio-structural research. In the end, researchers all across Europe were able to use over half a billion core

hours of computer simulations to fight the COVID-19 pandemic through the Call—time that amounts to over 57 000 years.

After working for over a year to establish urgent computer access, the PRACE committee in charge of assessing the proposals and allocating the HPC resources has condensed the key lessons stemming from the call, which will be useful as blueprints for the next fast-track program for crises situations. The key lessons are: ensuring the availability and openness of the produced data and related metadata; the encouragement of cross-disciplinary proposals, which would address the integrated, highly intertwined and cascading effects of a pandemic or other emergencies; the modification of the technical requirements to support proposals in scientific fields that are technically less prepared to run on HPC but are potentially useful to combat the pandemic or other crises; and the implementation of rigorous scientific peer evaluation to avoid proposals that won't be able to yield tangible results in the short term.

"The community has worked a lot on the COVID-19 Fast Track Call—everyone involved has been very generous with their time. It has been a very positive experience. Nevertheless, we need more people studying and working in technical areas, as this will allow us to have the best algorithms and use them efficiently when the next crisis arises," concludes Prof. López.

More information: Lessons learned from urgent computing in Europe: Tackling the COVID-19 pandemic, *Proceedings of the National Academy of Sciences* (2021). doi.org/10.1073/pnas.2024891118

Provided by Institute of Chemical Research of Catalonia