

## **Computers join the fight against COVID-19**

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Scientists everywhere are banding together to fight the novel coronavirus, and they're already making progress. Computational chemists are focused on building computer models of the virus's parts, which could aid in developing new therapeutics. Now, organizations around the world are offering up their computing power to researchers to



help provide rapid results, according to an article in *Chemical & Engineering News (C&EN)*.

Building an accurate model of SARS-CoV-2, the virus that causes the COVID-19 illness, requires a significant amount of <u>computing power</u>. This is especially true if scientists want fast results from their simulations, which is a given under current circumstances, writes Assistant Editor Sam Lemonick. In the U.S., a group of universities, national labs and corporations have formed a consortium offering free computing resources to researchers, including Google's and Amazon's extensive cloud services and some of the world's most powerful supercomputers. Similar efforts are underway in Europe, China and elsewhere, with the goal of providing rapid resources for an ever-evolving situation.

To take advantage of these resources, researchers submit proposals to the consortia, which are then fast-tracked for approval. Although many scientists who request computing resources are familiar with these technologies, the U.S. and E.U. consortia plan to assist those who aren't by matching them with expert collaborators. Current projects include a study on protein inhibitors of viral enzymes that could prevent SARS-CoV-2 from replicating, using powerful supercomputers from Oak Ridge National Laboratory. The consortia are looking for scientists in a broad range of dis ciplines to use these computer systems for fighting COVID-19. Researchers are encouraged to keep submitting proposals, with the hope that the sense of urgency will lead to real progress in the near future.

More information: <u>cen.acs.org/physical-chemistry</u> ... <u>s-fight-</u> <u>COVID/98/i15</u>



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