

FROM QUARKS TO CORONAVIRUS:

Computing the Building Blocks



The supercomputers at the Department of Energy's Thomas Jefferson National Accelerator Facility (Jefferson Lab) are typically focused on calculating the building blocks of matter. But now, those same machines are calculating the building blocks of the COVID-19 coronavirus. Portions of the Jefferson Lab supercomputers are now dedicated to combat the virus by supporting the Folding@home project, which is modelling the proteins that make up COVID-19.

The Folding@home project simulates protein dynamics, specifically how a protein's components are arranged and how they move. Viruses, including COVID-19, contain proteins

that may suppress our immune systems and that help the virus reproduce. Folding@home takes advantage of compute time donated by citizen scientists and organizations to run simulations of these proteins. It is currently simulating the dynamics of COVID-19 proteins to aid in the hunt for new therapies to combat the virus.

Recently, the Folding@home project requested donations of compute time on GPUs to support COVID-19 researchers. Jefferson Lab's supercomputer clusters are powered by two different technologies: traditional central processing units (CPUs) and newer graphics processing unit (GPUs), such as those

found in home gaming consoles. Jefferson Lab answered the call by making time available on two of its GPU supercomputers and by ensuring that the Folding@home project code could run successfully on the computer systems. The laboratory also dedicated additional resources to the effort on its CPU-based supercomputers.

This donation of computing resources is making an impact for the Folding@home project, with no negative impacts on the laboratory's own experimental program. Jefferson Lab's contribution to the COVID-19 effort can be tracked here: <https://stats.foldingathome.org/donor/74588160>

Jefferson Science Associates, LLC, a joint venture of the Southeastern Universities Research Association, Inc. and PAE, manages and operates the Thomas Jefferson National Accelerator Facility, or Jefferson Lab, for the U.S. Department of Energy's Office of Science.

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