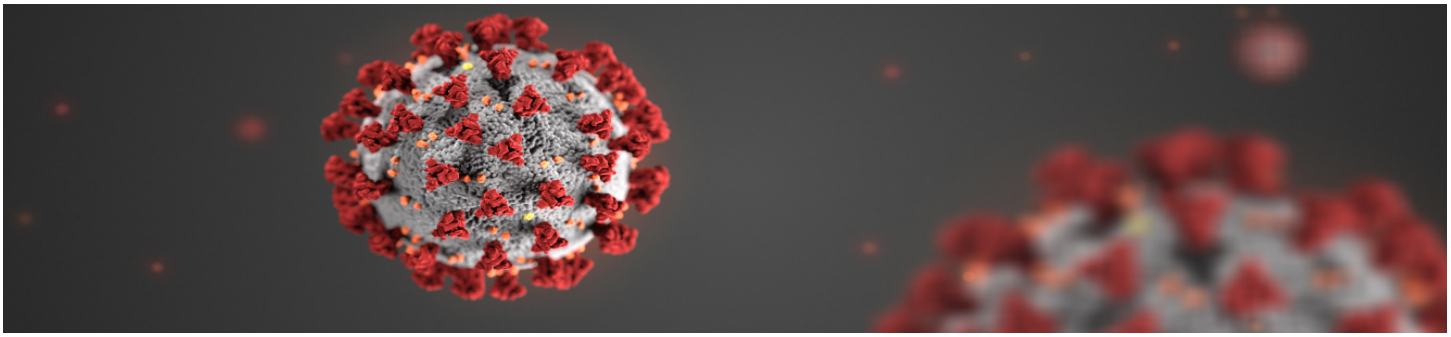
Harnessing Computing Power to Fight COVID-19



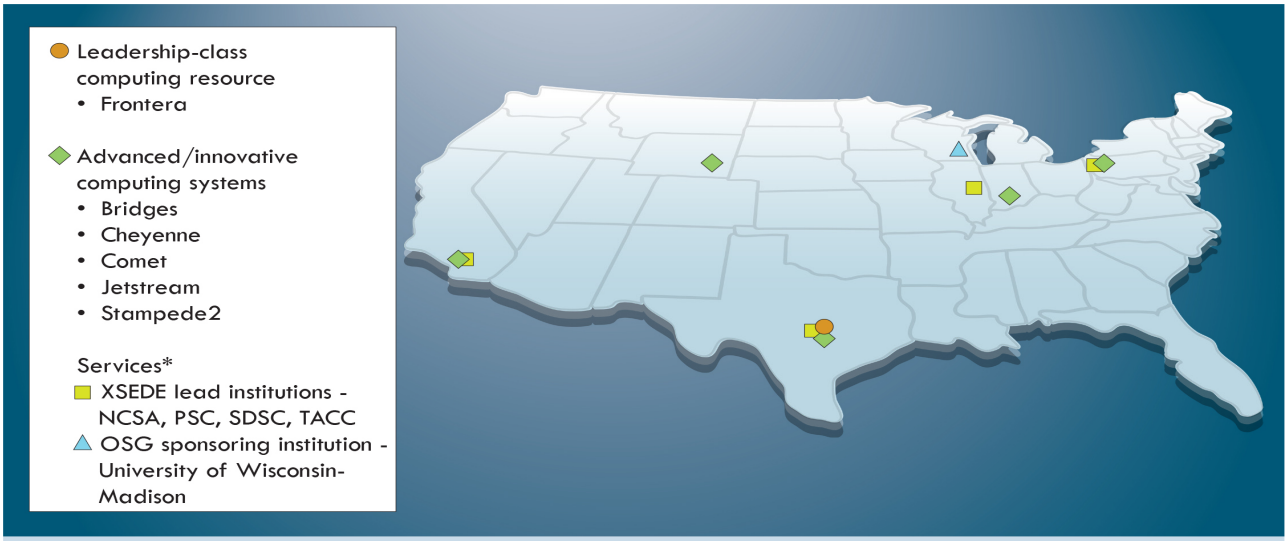
COVID-19 HIGH PERFORMANCE COMPUTING (HPC) CONSORTIUM

- March 23, 2020 - The White House announced the launch of the COVID-19 High Performance Computing (HPC) Consortium, a unique public-private consortium spearheaded by the White House Office of Science and Technology Policy, IBM, the National Science Foundation (NSF), and the U.S. Department of Energy. The HPC Consortium enables researchers to access the most powerful high-performance computing resources to accelerate understanding of the COVID-19 virus and develop methods for combating it.
- For over four decades, NSF has been at the forefront of advanced computing capabilities, providing researchers across the country access to computing systems that are key to keeping the U.S. a global leader in research and education.

Providing access to **30 supercomputing systems, 402 petaflops, 105,334 nodes, 3,539,044 CPU cores, 41,286 GPUs,** and counting...

- NSF-supported computing systems powering the HPC Consortium include: the leadership-class computing resource, Frontera, at the Texas Advanced Computing Center (TACC); Bridges at the Pittsburgh Supercomputing Center (PSC); Cheyenne at the NCAR-Wyoming Supercomputing Center; Comet at the San Diego Supercomputer Center (SDSC); Jetstream at the Indiana University Pervasive Technology Institute (PTI); and Stampede2 at TACC.
- NSF-supported services, the Extreme Science and Engineering Discovery Environment (XSEDE) and the Open Science Grid (OSG), are also working to integrate and coordinate resources available to the HPC Consortium.

MAPPING NSF'S COMPUTING POWER



NSF-funded advanced computing systems and services enabling the COVID-19 HPC Consortium.
*XSEDE is a collaborative partnership of 19 institutions, and OSG has more than 100 active virtual organizations worldwide.

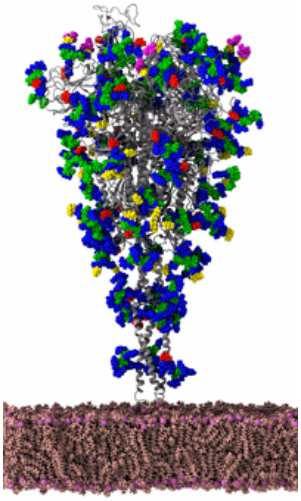
- Powerful data analytics, machine learning, artificial intelligence, and other advanced computing capabilities available through NSF-supported computing resources are giving rise to new knowledge and discovery not otherwise possible. These systems contribute to the Nation's economic competitiveness and security, and in the current environment, they are critical to advancing researchers' understanding of COVID-19.

SIMULATIONS TO UNDERSTAND TRANSMISSIBILITY

- NSF-funded advanced computing systems have been supporting University of California-San Diego Chemistry and Biochemistry Professor Dr. Rommie Amaro's work to understand the transmissibility of influenza viral infections since 2014.
- As recently as February 2020, the Dr. Amaro's research has advanced our understanding of the transmissibility of the H1N1 Influenza virus, enabled by simulations on the Blue Waters supercomputer at the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign. This research was instrumental in allowing a quick response to the COVID-19 crisis.
- The Frontera team at TACC provided considerable support in March 2020 in terms of expertise in benchmarking, porting, and scaling the code to enable large-scale runs on the Frontera system. The simulations utilized 4,000 nodes, or about 250,000 processing cores, which amounts to half the total computation capability available on the system.
- Dr. Amaro's lab built on experimental cryogenic electron microscopy (cryoEM) research from University of Texas at Austin that illuminated the near-atomic resolution structure of the SARS-CoV-2 spike proteins, the most important viral protein involved in infecting host cells. Through her simulations on Frontera, Dr. Amaro is leading the effort to build the first complete all-atom model of the SARS-CoV-2 envelope. This effort is critically important to understanding the viral protein used by COVID-19 to infect host cells and crucial to understanding how best to react to this new threat.

#1 Frontera is the most powerful academic supercomputer in the world.

#5 Frontera is the fifth most powerful supercomputer in the world.



SARS-CoV-2 spike protein of the coronavirus as simulated by the Amaro Lab on the Frontera system.

SUPPORTING COLLABORATIVE RESEARCH

- Dr. Amaro's work in response to the COVID-19 crisis is also a demonstration of the national collaborative research enterprise between NSF and the National Institutes of Health (NIH). The Amaro lab's scientific research in developing and applying state-of-the-art computational and theoretical techniques to the investigation of biological systems is funded by NIH. Access to the Frontera supercomputer and the development of the system itself was made possible by NSF's investment in leadership-class computing resources.

DID YOU KNOW?

According to *Encyclopedia Britannica*, the term "supercomputer" is commonly applied to the fastest high-performance systems available at any given time. Such computers have been used primarily for scientific and engineering work requiring exceedingly high-speed computations. Frontera was named the #5 top supercomputer in the world and #1 academic supercomputer in the June 2019 rankings of the Top500 organization.

Coronavirus.gov **Coronavirus Disease 2019 (COVID-19)** **What the U.S. Government is Doing**

Image credits: Page 1 Centers for Disease Control and Prevention (CDC) Page 2 (top to bottom) TACC; TACC and Rommie Amaro, UC San Diego