



NSF-SUPPORTED SUPERCOMPUTERS BUILD ON PANDEMIC RESPONSE EFFORTS

Expanding COVID-19 Work and Addressing Other Potential Pandemics

Covid-19 High Performance Computing (HPC) Consortium Adds Resources

THE COVID-19 HIGH PERFORMANCE COMPUTING (HPC) CONSORTIUM was launched in March 2020 to combine the computing resources of federal agencies, industry and academia to enable researchers to access the most powerful high-performance computing resources and better facilitate COVID-19 research and the fight to stop the virus. Building on 40 years of supercomputing development and support, the **U.S. National Science Foundation** is a key member of the public-private consortium, working with the **White House Office of Science and Technology Policy**, **IBM** and the **U.S. Department of Energy** to launch and support the project.

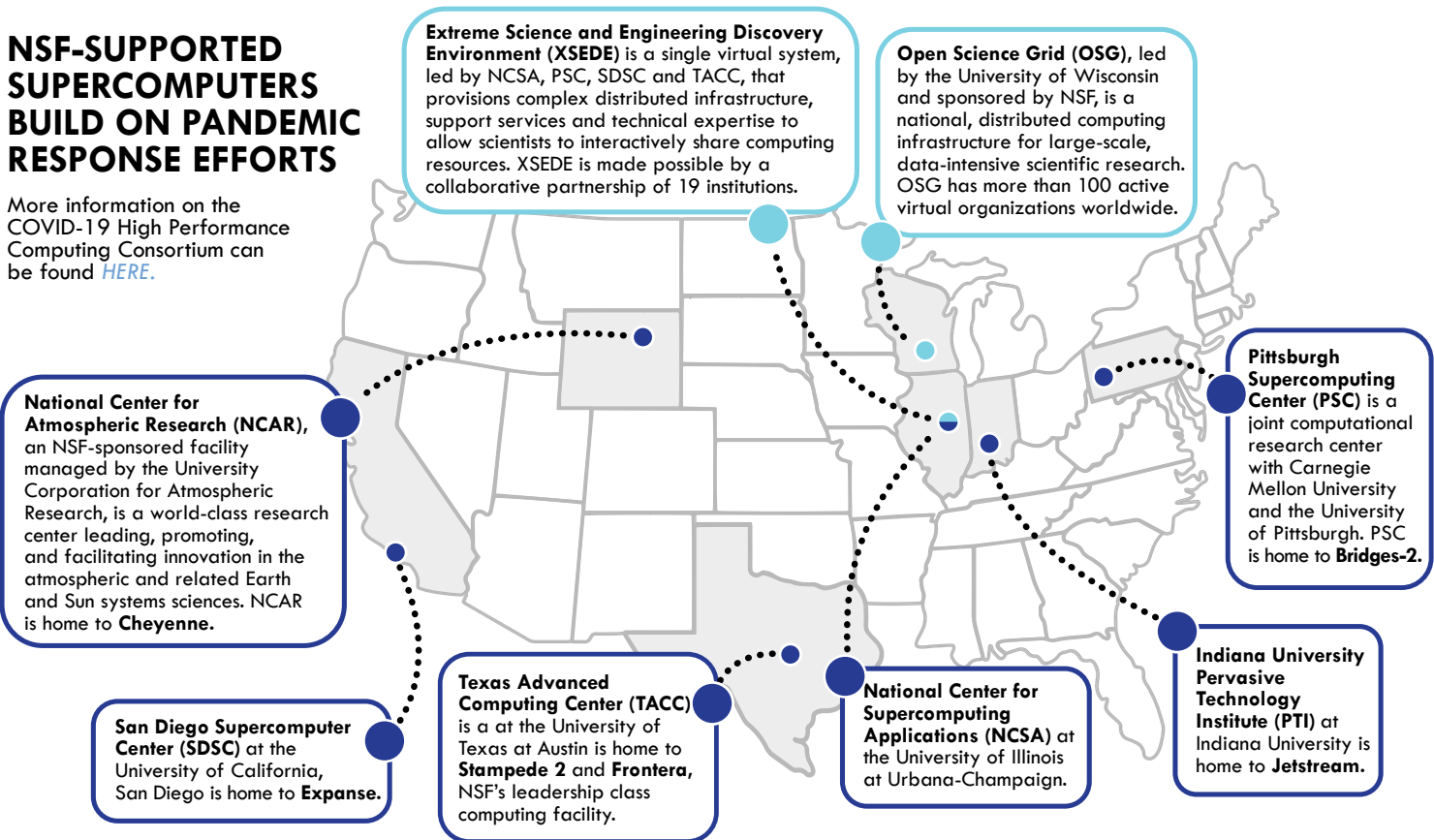
NSF-supported computing systems powering the HPC Consortium include: the leadership-class computing resource, **Frontera**, at the **Texas Advanced Computing Center (TACC)**; **Bridges**, at the **Pittsburgh Supercomputing Center (PSC)**; **Cheyenne**, at the **NCAR-Wyoming Supercomputing Center**; **Expanse**, at the **San Diego Supercomputer Center (SDSC)**; **Jetstream**, at the **Indiana University Pervasive Technology Institute (PTI)**; and **Stampede2**, at **TACC**.

The HPC Consortium now includes **43 Members** (many international), **600 Petaflops** of computing power (up from 330 at launch), **50,000 GPUs**, **165,000 Nodes**, **6.8 Million Cores** – allocating those resources to more than 100 projects.

The NSF-supported **Extreme Science and Engineering Discovery Environment (XSEDE)** serves as the hub for the HPC Consortium. The NSF-supported **Open Science Grid (OSG)** is also working to integrate and coordinate resources available to the HPC Consortium.

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More information on the COVID-19 High Performance Computing Consortium can be found [HERE](#).



Early Successes Helped Accelerate Vaccine Developments

PHASE 1 OF THE HPC CONSORTIUM focused on understanding the virus, tracking the spread and developing treatments and vaccines. NSF supported hundreds of projects.

Rommie Amaro, a computational biophysical chemist at the **University of California, San Diego**, built a model of the exterior structure of the SARS-CoV-2 coronavirus, using **Frontera** to model how it binds to human cells. The simulations revealed that molecules called glycans help the virus bind to receptors on human cells. Identifying this activity helped accelerate the development of new treatments. In recognition of this work, **Amaro** and her team received the **ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research** in November 2020.

Amanda Randles, a biomedical engineer at **Duke University** and an *NSF career awardee*, developed a ventilator splitter and resistor system to help address the shortage of these life-saving machines at hospitals. To complete the simulations needed to develop the device, the **HPC Consortium** matched **Randles** and her team with Microsoft to run the computations on the **Azure HPC**. Thousands of hours of work was completed in a single weekend and the system was approved for emergency use in September 2020 by the **U.S. Food and Drug Administration**.

Ashok Srinivasan, a computer scientist at the **University of West Florida**, used **Frontera** to study how to mitigate the risk of the virus spreading in constrained physical environments, such as an airplane cabin. The research simulated different methods used to board passengers and found that boarding aircraft back to front increases the risk of exposure compared to random boarding because of the increased clustering of passengers. Srinivasan has conducted research on the risk of COVID-19 in crowded locations under an *NSF RAPID award*.

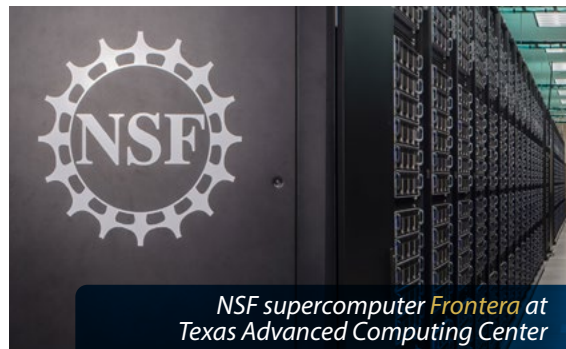
Madhav Marathe, a computer scientist at the **University of Virginia's Biocomplexity Institute**, led a team of researchers across 14 U.S. institutions that harnessed the power of **Big Data** computing to plan for and respond to outbreaks such as COVID-19. The team used resources such as **Bridges** to study how complex networks of human behavior affect the virus's patterns of transmission. Their findings helped decision makers at several institutions and health agencies understand and manage the epidemic as well as predict future outbreaks.

Increase in Available Data Fuels New Research Phase

IN NOVEMBER, THE HPC CONSORTIUM ANNOUNCED IT WOULD MOVE TO PHASE 2, focusing on benefiting patients in the near term and on scientific breakthroughs in the long term. Building on the volume of COVID-19 data now available, research includes understanding and modeling patient response to the virus, validating vaccine response models from multiple clinical trials, evaluating combination therapies and designing epidemiological models driven by large datasets.

Creating the National Strategic Computing Reserve

THE QUICK DEPLOYMENT AND SUCCESS OF THE HPC CONSORTIUM in addressing the COVID-19 pandemic demonstrated the valuable role that supercomputing resources can play in response to national emergencies. The members of the public-private partnership are now seeking input on the creation of a **National Strategic Computing Reserve (NSCR)**, a coalition of experts and resource providers that could be mobilized quickly to provide computational resources in times of urgent need. Scientists and engineers envision that the benefits of NSCR would extend beyond pandemics to also address emergencies resulting from natural and man-made disasters as well as broader issues such as climate change.



Work on COVID-19 using NSF-supported supercomputers continues today:

Bridges –

A team from **Carnegie Mellon University** developed a new computational pipeline for speeding up the identification of possible anti-COVID-19 candidates using artificial intelligence (AI) on the XSEDE-allocated **Bridges-AI** system. They used this tool to screen about 5 billion chemical compounds thousands of times faster than possible with previous models and selected a small number of candidates for combating the disease.

Cheyenne –

A consortium of researchers used **Cheyenne** to study how changes to the emission of particulates (aerosols) affect climate, using estimates of emission changes for 2020 in two climate models to simulate the impacts of the COVID-19-induced emission changes.

Expanse/Stampede2 –

University of New Hampshire researchers used **Expanse** and **Stampede2** to identify new inhibitor pathways in an RNA-based virus. The findings could help understand how these inhibitors react and could potentially help develop a new generation of drugs to target viruses with high death rates, such as HIV-1, Zika, Ebola and SARS-CoV-2. Researchers ran hundreds of simulations at the same time to observe what are called rare base-flipping events involved in the inhibitor binding/unbinding process that provided the new details of the underlying mechanism behind this process.

Frontera –

An NSF supplemental award and contributions from Dell Technologies and Intel funded an expansion of **Frontera**, adding nearly 3.5 million node hours of compute time to focus on urgent computing capabilities. In April, NSF approved allocations of time on Frontera for 58 projects, including research by the University of Arkansas to determine the differences in behavior of spike protein structure of SARS-CoV-1 and three different variants of SARS-CoV-2 with different transmission levels.

