



# Oak Ridge Leadership Computing Facility

## Breakthrough Science at Every Scale

Simulation is a vital part of the research process, joining theory and experiment to form the three pillars of science. With simulation, researchers have the ability to study extreme-scale phenomena such as climate cycles all the way down to the most microscopic of materials. The Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory is one of the most powerful high-performance computing (HPC) centers in the world, providing researchers working on some of the most challenging problems of the 21st century with leadership-class computers for scientific simulations.

These HPC systems—supercomputers—enable a level of detailed analysis unavailable through traditional experimental or theoretical means. Coupled with the expertise of the OLCF technical staff, supercomputers such as the ones at the OLCF afford scientists new opportunities to study subatomic particle interactions, simulate the volatile conditions inside a combustion or turbine engine, develop new treatments for diseases, design materials that can revolutionize industries, and model the origins of the universe.

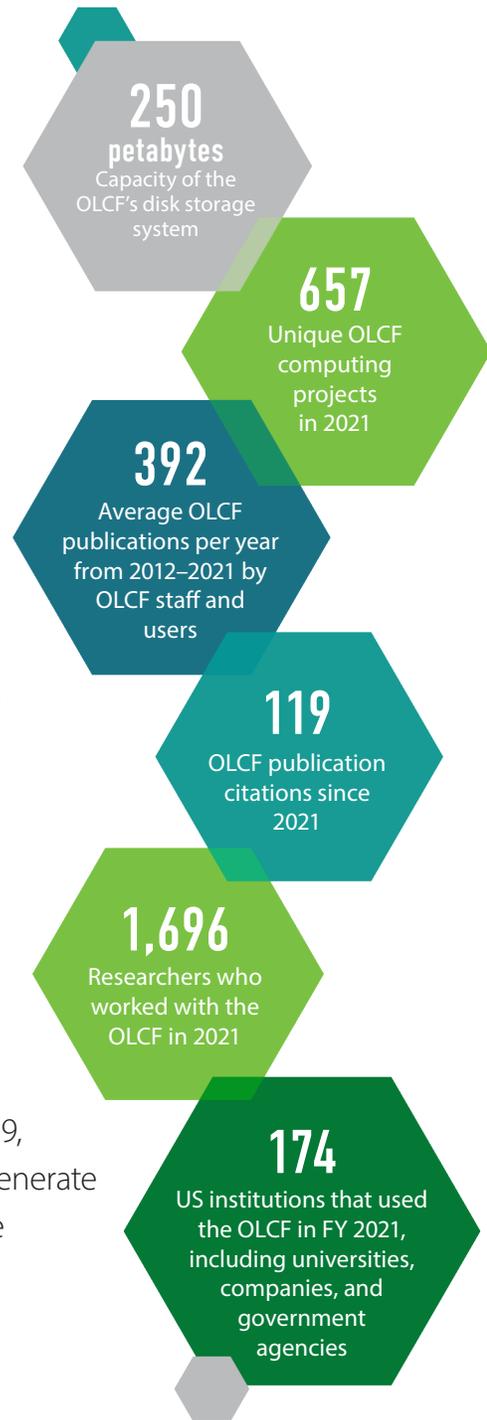
## Supercomputers for Speedy Solutions

The OLCF is home to the nation's fastest supercomputer, Summit, an IBM AC922 system that debuted in 2018. Summit has a theoretical peak performance of 200 petaflops, meaning the system can solve 200 quadrillion calculations per second. Summit is about eight times more powerful than its predecessor, the OLCF's previous 27-petaflop Titan supercomputer.

With Summit and other HPC resources at the OLCF, scientists can employ more precise calculations and develop increasingly complex models, leading to high-fidelity solutions. In 2018, researchers broke the exascale barrier on Summit with a genomics algorithm, achieving a peak throughput of 2.36 exaops—or 2.36 billion billion reduced precision calculations per second, the fastest science application ever reported. The next chapter in the OLCF's legacy is taking shape in the form of Frontier, which is slated to be the nation's first exascale system with a sustained speed of greater than 1.5 exaflops when it comes online for early users in 2022.

"To draw scientific conclusions in our work related to COVID-19, we need to run many molecular dynamics simulations and generate an enormous amount of data. Summit provides the immense compute power to handle that workload."

**John Gounley, Summit User  
and Computational Scientist, ORNL**



# Recent Impacts

**Industrial competitiveness**—General Electric uses Summit to simulate combustion in gas-powered turbines. By using computer simulations, researchers get more designs to evaluate, allowing them to make leaps in turbine efficiency that translate to millions of dollars in saved fuel and millions of tons of reduced carbon pollution.

**Energy-efficient materials**—A team at Lawrence Berkeley National Laboratory is using Summit to study copper-based superconductors to understand the interactions between the particles in these materials. Superconductors have zero electrical resistance when they reach sufficiently low temperatures and are being explored for technologies such as magnets for MRIs, fusion devices, and particle accelerators.

**Understanding COVID-19**—Researchers at Argonne National Laboratory have used Summit to simulate the SARS-CoV-2 virus' spike protein in numerous environments, including within the SARS-CoV-2 viral envelope comprising 305 million atoms—the most comprehensive simulation of the COVID-19-causing virus performed to date. The results have led to discoveries of one of the mechanisms the virus uses to evade detection as well as a characterization of interactions between the spike protein and the protein that the virus takes advantage of in human cells.

## Summit by the Numbers

<b>200 petaflops</b>	If everyone on Earth made one calculation per second, it would take more than 300 days to do what Summit can do in 1 second.
<b>8.8 megawatts</b>	Summit is very efficient, demonstrating a sustained performance of 122.3 petaflops using just 8.8 megawatts of power.
<b>4,000 gallons</b>	The amount of chilled water circulated through Summit every minute.
<b>5,600 square feet</b>	Summit's footprint is about as big as two tennis courts.

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