Lawrence Livermore National Laboratory Expands Corona Cluster to Perform Additional COVID-19 Research

Supermicro's GPU servers increase performance to 11 Petaflops

INDUSTRY
Science and Technology

Lawrence Livermore National Laboratory's (LLNL) mission is to strengthen the United States' security by understanding and reacting to threats. This mission includes identifying and applying state-of-the-art technology to reduce the risk to the US and the world from a range of possible scenarios.

In early 2020, the fast spread of the novel coronavirus that causes COVID-19 was quickly becoming a national security concern. Nobody understood the virus' biology, and treatments were non-existent. The United States government looked to its research institutions' network and moved rapidly to create or expand the computing infrastructure available for this unprecedented challenge.

CHALLENGE
- Fast deployment
- Latest Technology
- Rack Level testing

Challenge

With funding from the Coronavirus Aid, Relief, and Economic Security (CARES) Act, LLNL determined that one of these funds' best uses was to upgrade a supercomputer that could target the fight against COVID-19. The Corona server cluster (named for the "corona" of the sun visible during the solar eclipse in 2017) supported various open science research projects and was available to LLNL's network of researchers. However, with the urgency to understand and find a treatment for COVID-19, LLNL decided

to create a system focused on the simulation workloads to find therapeutics against the SARS-CoV-2 virus. Using Artificial Intelligence (AI) and Machine Learning (ML) algorithms, researchers believed a system with many GPUs would provide the right platform.

"One of the requirements for the fast deployment of the expanded Corona HPC system was that the vendor is able to deliver an integrated and tested rack of servers. This requirement was necessary to offer these new capabilities quickly to our worldwide community of COVID-19 researchers. Supermicro was able to deliver the state-of-the-art servers quickly, but also tested at the rack level."

–Trent D'Hooge, deputy division leader for operations, Livermore Computing

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LLNL faced several requirements when deciding to upgrade the Corona system. These included:

- Fast deployment—Researchers were eagerly waiting to use the additional compute capacity that the Corona system would contain.
- Appropriate Technology—LLNL wanted to use the latest CPUs from AMD due to their high number of cores and communication with a GPU.
- Powerful GPUs—The applications that LLNL needed to run on this system were heavily dependent on the availability of state-of-the-art GPUs
- Delivery of a fully working rack-level solution that would reduce the time to results.
- Learning to use and developing tools for future supercomputer class systems

LLNL researchers and others across the US were experts in creating COVID-19 antibodies and small molecule anti-viral medicines.

NODE SOLUTION

- Supermicro Server: A+ Server 4124GS-TNR 4U 8 GPU system

- 256 GB per node

Solution

Supermicro has been a supplier of advanced server solutions for many years. When the need came to acquire the latest in CPU and GPU servers quickly, LLNL immediately contacted Supermicro to determine what the most advanced AMD servers were available. LLNL decided that the AMD EPYC 7002 processors, combined with the AMD Radeon Instinct ™ MI50 GPU accelerators, were an excellent match for the molecular dynamics simulations critical to finding the free energy of binding between antibodies-antigens. ML algorithms were also employed to speed up identifying potential antibodies that could be artificially manufactured. These AI and ML algorithms are highly dependent on GPUs parallel nature and fast communication to and from the CPUs.

The Corona server cluster was expanded to include over 120 additional servers, which contained the AMD EPYC 7002 series CPUs and almost 1,000 AMD MI50 accelerators. Many ML and molecular dynamics applications took advantage of the high performant MI50 GPUs. Future work will focus on running large ensemble molecular docking and dynamics simulations using a wider range of CPU and GPU resources. The Corona system is designed with the Mellanox HDR-100 IB network.

The total peak computing performance of the expanded Corona system is 26.5 Teraflops when using half-precision floating-point numeric representation. When using single-precision representation, the theoretical peak performance is 13.3 Teraflops.

Corona is integrated into the LLNL simulation environment, including access to Lustre and VAST parallel files system and traditional network file systems.

Benefits

LLNL quickly upgraded its existing Corona HPC system so that additional research could be performed to find antibodies and other therapeutics for the devasting COVID-19 pandemic. The ability to quickly bring up a complex system was critical, as researchers were eager to increase application throughput for extensive ensemble simulations. Corona installation and acceptance went quickly and smoothly, with the system being fully subscribed by researchers within minutes of becoming operational.

Supermicro delivered fully functional racks, with all servers and networking switches tested, significantly reducing the time to bring up a system and start-up challenges. The new, updated system is rated at over 11 Petaflops of computing power, with the addition of 121 nodes, each with eight AMD MI50 GPUs.

In addition to use by LLNL scientists, the Corona system is also being made available to researchers worldwide through the COVID-19 High-Performance Computing Consortium. Researchers can apply to use the system, and experts at LLNL can quickly determine if the applications are tuned to this type of CPU and GPU system.

ABOUT SUPERMICRO

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