Accelerating scientific research with high performance computing

The Arizona State University Research Computing organization applies advanced computational resources to grand challenges in science, engineering and health.

Customer profile

Arizona State University

Scientific Research | United States

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Douglas Jennewein
Senior director of Research Computing
Arizona State University

Business needs

Researchers at Arizona State University need leading-edge HPC clusters to drive compute- and data-intensive research.

Business results

- Enabling groundbreaking scientific research
- Accelerating discovery and innovation
- Solving grand challenges in science, engineering and health
- Driving advanced computing forward for all users

Solutions at a glance

- Dell EMC PowerEdge servers with Intel® Xeon® processors
- GPU accelerators
- Dell EMC PowerScale Isilon scale-out network attached storage
- Intel® Omni-Path, InfiniBand and Ethernet fabrics
- Omnia and Open OnDemand software

A commitment to research

Scientific research has long been a core part of the mission of Arizona State University. Today, the university holds the distinction of being one of the fastest-growing research institutions in the United States. Since 2002, the school's annual research expenditures have more than quintupled, topping $600 million, and ASU is among the top 20 universities in the world for the number of U.S. patents issued.[1]

Under the umbrella of this vast research program, ASU scientists explore some of the world's most complex challenges, including those arising from population growth, urbanization, globalization and technological advancements. Through science, social science and humanities approaches, ASU researchers are creating innovative and sustainable solutions to pressing societal problems.

Many of these research initiatives would not be possible without the computational power of high performance computing, and this is where the ASU Research Computing organization enters the picture. ASU Research Computing is dedicated to enabling research, accelerating discovery and spurring innovation through the application of advanced computational resources to grand challenges in science, engineering and health.

The HPC environment

Among other resources, ASU Research Computing gives the university community access to a Dell Technologies supercomputing cluster that comprises 14,000 CPU cores, 330 GPU devices, 1.2 petabytes of scratch storage in a high-speed parallel file system and 4 petabytes of Dell EMC PowerScale Isilon scale-out network attached storage.

1 Arizona State University, "Research and innovation at Arizona State University," accessed March 23, 2021.

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> senior director of ASU Research Computing

This highly heterogenous environment includes a mix of CPUs, including multiple generations of Intel® Xeon® processors, a variety of interconnects, including Intel® Omni-Path, InfiniBand and Ethernet fabrics, and a range of Dell EMC PowerEdge servers. It also includes dedicated virtual machines for specific research environments and a HIPAA-aligned secure computing environment with support for sensitive or federally regulated data.

System users have two ways to access the supercomputing cluster, according to Douglas Jennewein, Senior Director of the Research Computing group at ASU. Users can log in to the cluster via a traditional SSH terminal or via a web-based interface that uses Open OnDemand, an open-source HPC portal based on software developed by the Ohio Supercomputer Center.

With Open OnDemand, users can upload and download files; create, edit, submit and monitor jobs; run applications; and more, all via a web browser, with no client software to install and configure. The result is a cloud-like feel to the process of accessing and using HPC resources.

"Open OnDemand is a very popular access modality for our researchers," Jennewein says. "It has really been a game changer for us."

Easy access to the cluster via Open OnDemand has fueled a rush on resources.

ASU Research Computing now accommodates many more users than in the past, including large numbers of academics from disciplines that typically aren't associated with advanced computing. In a parallel change, ASU Research Computing is increasingly serving faculty members who are using the HPC cluster in the classroom, along with growing numbers of student users.

Usage numbers tell the tale of the popularity of the HPC cluster. Over the past year, ASU Research Computing has delivered an average of 8 million core CPU hours per month. In any given month, 500 to 600 users put the system to work, and over the course of a year 1,300 distinct users make use of the system. The HPC cluster typically runs about half a million jobs per month.

"Open OnDemand, the web-based access, has opened up a whole new class or segment of users, folks who are newer to the cluster or newer to advanced computing," Jennewein says. "This is a much more friendly onramp to HPC than traditional approaches. This has opened up the door for a lot more use cases and domains of science and research that are traditionally under-represented in high performance computing, including humanities, social sciences and the arts."

Fueling discovery and innovation

The resources delivered by ASU Research Computing enable a range of research initiatives that are as diverse as the academic domains of a university. Increasingly, these initiatives incorporate HPC-driven techniques for data analytics, machine learning, deep learning and artificial intelligence. From sequencing genomes to analyzing imagery captured by scientific instruments, from evaluating drug interaction to modeling power grids, the research now depends on the computational power of a supercomputer.

"When we think about the kinds of computation that HPC enables, we think about things that are either very big or very fast," Jennewein says. "These are things that simply cannot be conducted on a laptop or a desktop because there's not enough RAM or there's not enough CPU or there's not enough storage. These are the kinds of problems that we lend ourselves well to."

One of the current areas of emphasis is research focusing on the SARS-CoV-2 virus and the deadly COVID-19 disease.

"We have several researchers involved in COVID-related research on the system," Jennewein says. "The ability of ASU researchers to contribute to the national and global fight against COVID is catalyzed and enabled by advanced computing. For example, we have researchers looking at the molecular dynamics of protein and virus interactions with potential drugs. That is something that you just can't do without HPC."

When he reflects on the value brought by ASU Research Computing, Jennewein talks about the importance of making HPC available to an ever-widening pool of researchers and about helping scientists focus more on their science and less on the enabling technologies.

"Perhaps at the highest level, we are a technology organization that is dedicated to giving minutes back to science," he says. "We can't change the nature of computing, but we can help folks compute as fast as possible, to reduce time to discovery and accelerate the pace of science."

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An HPC & AI Center of Excellence

Arizona State University is among an elite group of Dell Technologies HPC & AI Centers of Excellence. These centers, found around the world, provide thought leadership, test new technologies and share best practices with technology users. They offer collaborative expertise that spans from high-speed data analytics, AI, machine learning and deep learning to visualization, modeling, simulation and more. They also engage in performance analysis, optimization and benchmarking, along with system design, implementation and operation.

Jennewein notes that as an HPC & AI Center of Excellence, ASU has access to Dell Technologies' deep bench of HPC expertise, engineers and integration approaches.

"Having access to that deep bench has been incredibly valuable to us," he says. "We often collaborate on proposals. For example, we recently worked with Dell to put in a National Science Foundation proposal on integrating dense GPU systems in an existing cluster environment. That would be transformational for us, to have a newer, smarter way of delivering GPU computing."

Among other recent joint efforts, ASU Research Computing is working closely with the Dell Technologies HPC & AI Innovation Lab on the development of the Omnia software stack. This open source community project helps HPC shops speed and simplify the process of deploying and managing environments for mixed workloads, including simulation, high throughput computing, machine learning, deep learning and data analytics.

"We have ASU engineers on my team working directly with the Dell engineers on the Omnia team," Jennewein says. "We're working on code and providing feedback and direction on what we should look at next. It's been a very rewarding effort. Omnia is something we want everybody to use. We're paving not just the path for ASU but the path for advanced computing."