

SDSC EXPANDS ACCESS TO SCIENTIFIC DISCOVERY WITH AMD

SDSC CASE STUDY

SDSC broadened research access to high performance computing resources by deploying AMD EPYC™ processors



The San Diego Supercomputer Center (SDSC) has been harnessing the capabilities of AMD EPYC™ processors for scientific research for the last four years. The CPUs have enabled SDSC to expand its supercomputing science to a wider range of researchers. Now, the Center is about to broaden its offering with AMD Instinct™ APU, for an even wider community of research, including AI.

“We’re one of the original supercomputer centers funded by the National Science Foundation,” says Robert Sinkovits, Ph.D, Project Manager, Expanse Supercomputer, SDSC. “We go way back to 1985. We serve more than a thousand researchers covering 300 universities across the United States. We have physicists, molecular biologists, humanities, social sciences, and earth sciences.”

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Robert Sinkovits, Ph.D, Project Manager,
Expanse Supercomputer, SDSC

“A big part of our user base is researchers from life sciences,” says Sinkovits. “We have a large user base that is interested in cryo-electron microscopy. We support phylogenetic inference, constructing trees of life from genomic data. We support the physical sciences, including astronomy and astrophysics. Recently, we worked with a research group that was making predictions of what the solar corona would look like during the 2024 eclipse, and they were very close to reality. We have many researchers from computational chemistry and material sciences who are looking at developing new materials for energy applications. There’s a lot of work in computational chemistry.”

WIDENING ACCESS WITH SCIENCE GATEWAYS

However, one of the key innovations at SDSC is how it makes HPC resources more widely available to researchers. “We are one of the pioneers of science gateways,” says Sinkovits. “These are like a Web interface to a supercomputer. Not everybody wants to write their own parallelized applications using Message Passing Interface (MPI) and OpenMP. With the science gateways, we install the software on the supercomputer and make it available through sophisticated Web interfaces so that users can upload their data sets. They can still do their calculations, but they are abstracted away from all the details of compiling and building codes, figuring out the number of cores or GPUs or processes to run on.

INDUSTRY

Higher Education | Research
High Performance Computing

CHALLENGES

Provide AI and high-performance computing resources to a wider range of scientific researchers

SOLUTION

Expanse supercomputer with AMD EPYC™ processors

RESULTS

Easier access to AI/HPC resources for researchers via science gateways without the need to code applications using MPI or OpenMP

AMD TECHNOLOGY AT A GLANCE

AMD EPYC processors

TECHNOLOGY PARTNER

DELL Technologies

Our most successful gateway, which has enabled more than 5,000 publications, is the CIPRES Gateway for constructing phylogenetic trees. These show the relationship between organisms, such as humans being closely related to bonobos and chimpanzees. That used to be done by zoologists. Now it's done using genomic data, and it's much faster and more accurate."

The primary supercomputer supporting these gateways is Expanse. "It is supported by the National Science Foundation and has been in operation for four years," says Sinkovits. "Dell Technologies, our integrator, incorporated over 1,400 2nd Gen AMD EPYC™ processors. We've expanded the system a few times and peak performance is now up to seven petaflops, so it's very powerful. AMD EPYC processors have been phenomenal. It was a game changer going from CPUs that had fewer cores to EPYC."

Our CPUs have 64 cores, and they are dual-socket servers, so we get 128 cores in a node. That is more than enough parallelism for many applications, so it has really democratized computing for us."

RESEARCH EMPOWERED BY MORE CPU CORES

"Each time we get a new supercomputer, it opens new horizons," says Sinkovits. "Going from Comet, our previous supercomputer, to Expanse, one of the biggest factors was the EPYC processors. Being able to get that many cores on a single chip facilitates so many users who were limited in how far they could go with their parallelism. If we have more cores within a node, we don't need to use MPI to go across multiple nodes. That has really accelerated research for a lot of our users who are in the long tail of science, needing anywhere from a handful to a few hundred cores. It's also been a real boon for our science gateways."

"The most exciting thing is that we can now support the entire academic research community," says Sinkovits. "It's thrilling when we get researchers from a new domain. When I started at the Supercomputer Center many years ago, we had a much more limited set of users, focused on the hard sciences—physics, chemistry, astronomy, astrophysics."

"Since Expanse arrived, we've had a lot more adoption by life science users, but we'll even see folks from sociology, anthropology, art, and music. I'm really thrilled when we get somebody new, who hadn't been using supercomputers before, or maybe they were doing computing at a much smaller scale on their laptop and now they can graduate to a larger resource."

LOOKING TOWARD THE APU FUTURE

"The AMD EPYC processors have been fantastic," says Sinkovits. "They opened so many new horizons by having that many cores on a CPU. The AMD roadmap already has 96-core processors, and 128 cores tuned for cloud workloads. We're excited about getting even more cores into a node. That will enable larger scale parallel computing for those who didn't make the leap to using MPI." AI will be another addition to SDSC's menu of possibilities. "We're going to see a lot more integration between traditional HPC and AI, where a component of the calculation that's well-suited for AI is going to be part of a larger simulation."

"This is where AMD Instinct™ APUs will soon be taking SDSC up yet another level. "I'm very excited about this move toward APUs," says Sinkovits. "The Cosmos system is going to be deployed very shortly at SDSC powered by AMD Instinct MI300A APUs, which is the first APU that has unified memory across the CPU and the GPU. That's going to enable so many more users to take advantage of accelerators."

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"When we just had straight GPUs, it was a very big lift to go from CPU to GPU," continues Sinkovits. "You needed to do a lot of work at a very low level with the memory management. APUs make it easier. Even for those who already know what they're doing, it will improve performance because they're not spending so much time moving data back and forth between the CPU and the GPU memory."



SDSC's new Cosmos supercomputer, powered by AMD Instinct MI300A APUs, will enable researchers to exploit powerful accelerator technology to aid their discoveries in AI, astrophysics, genomics, large language models, materials science, and many other domains.

“At SDSC, we are excited to be supporting researchers from any domain of research,” says Sinkovits. “If you’re doing open research, we want you to come here and not feel that you’re too small. We’re here to serve everybody, and we are particularly eager to help the folks who have not been doing supercomputing before. If you want to take the leap from your laptop or desktop to large-scale computing, come talk to us.”

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Expanse Supercomputer, SDSC



The Expanse supercomputer helped researchers better understand the sun's corona.



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ABOUT SAN DIEGO SUPERCOMPUTER CENTER

The San Diego Supercomputer Center (SDSC), located at UC San Diego, is a world-renowned leader in high-performance computing. SDSC provides cutting-edge computational resources, massive data storage systems, and expert consulting to researchers across diverse disciplines, including science, engineering, and medicine. Its advanced infrastructure enables large-scale simulations, complex data analysis, and groundbreaking scientific discoveries. SDSC plays a vital role in advancing research across numerous fields, from climate science to genomics. For more information visit expansion.sdsc.edu.

ABOUT AMD

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