Architecting for Mixed Workloads at Massive Scale

San Diego Supercomputer Center’s ‘Expanse’ supercomputer shows the way to optimal system balance.

Business needs

The San Diego Supercomputer Center at the University of California San Diego needs to bring balanced high performance computing resources to tens of thousands of academic- and industry-based researchers from across the United States.

Solutions at a glance

- Dell EMC™ PowerEdge™ servers
- NVIDIA® GPU accelerators
- AMD EPYC™ processors
- Mellanox® HDR InfiniBand

Business results

- Making HPC accessible to tens of thousands of users
- Supporting widely diverse workloads in a single HPC environment
- Accelerating scientific discovery in academic and industrial domains
- Unlocking the power of data to solve pressing human challenges as identified by the National Science Foundation

The new Expanse supercomputer is projected to have a peak performance of 5 petaflops. The Expanse supercomputer is expected to serve more than 50,000 users.
The case for carefully balanced supercomputers

The most important word in supercomputing systems architecture this decade will be balance. As workloads diverge, datasets grow in volume, compute demands become more challenging and the options for acceleration grow, system architects have a wide array of options. Ultimately, it takes detailed workload profiling to find a starting point. Today, we’re at this starting point. The large machines coming online show careful considerations have been made, which creates a diverse lineup of new supercomputers featuring specific choices in processors, accelerators, memory and storage profiles, and systems software features.

Building balanced high performance computing (HPC) systems is tricky because there is no one-size-fits-all approach for most sites. Each supercomputing site has to perform detailed analysis of current workloads, as well as project into the future to determine which future applications might place new demands on a system. The even-trickier part is that most HPC systems are procured years before they arrive, which makes the task of future-proofing machines even more challenging.

These considerations are even more difficult for sites that purchase massive-scale supercomputers that are geared to suit thousands of different users and applications, most with smaller or modest-sized jobs. Unlike some of the largest large-scale systems that have vast parallel jobs that often take over all or a significant part of the machine, broad scientific computing centers have to build balanced systems that have something for everyone, both for those with scalable applications and users who need to grab a few cores at a time.

Creating this complex large-scale system balance for a vast, diverse set of end users, all within the constraints of efficiency, performance, scalability and operational costs, falls to HPC center directors. Using workload profiles, lessons learned from past systems and broad industry insight, they are tasked with making decisions that must provide all stakeholders with the right machine. This is no small feat, according to Shawn Strande, deputy director of the San Diego Supercomputer Center (SDSC). Yet with help from his onsite teams, Strande and his colleagues have been able to weigh tradeoffs for the benefit of the widest number of end users possible with their new Expanse supercomputer, set to come online for thousands of scientific computing applications in 2020.

Serving the ‘long tail of computing’

“We are focused on the long tail of computing here at SDSC,” Strande explains. “We have a very large community of users running relatively small or modest jobs, which puts pressure on the system to deliver to highly mixed workloads, and a lot of work on the staff to support it. It’s the diversity of users and their application workloads that is one of the biggest challenges for a center like SDSC and for a system like Expanse.”

In terms of workload diversity, SDSC runs everything from high-throughput jobs from across scientific domains to Open Science Grid workloads (which total tens of thousands of single-core jobs). SDSC also handles near real-time analysis of experimental data from the LIGO Gravitational Wave Observatory as well as the expected batch scheduled jobs familiar in most research HPC environments. Science gateways for a wide range of academic areas have added more requirements for support, and naturally, the anticipated large GROMACs, NAMD and other big community codes must also run efficiently and scale well. SDSC has also had to fine-tune to be able to allow cloud-bursting when necessary in addition to providing the tooling needed for system composability. Supporting all of these workloads and usage models has taken great effort on the entire infrastructure stack, from hardware decision-making to systems software backbones.

“Our approach to system architecture is to start with a thorough understanding of our current workloads, add to that where we see emerging needs in the community, and within the constraints of fixed funding from the National Science Foundation for the system develop a design that gives users as much compute as possible, simultaneous with one that will achieve high levels of utilization while addressing the workloads,” Strande says. “Our processor selection, interconnect design, data elements (like local NVMe on all nodes, both a Lustre and object storage system), and software environment are the outcome of a deep understanding of the community, and a collaborative process with our vendor partner, Dell Technologies.”

“Expanse was a response to an NSF call for a capacity system that would serve research workloads across virtually all domains of science and engineering,” says Shawn Strande, Deputy Director, San Diego Supercomputer Center. “Collectively, we refer to these five modalities as the ‘long tail of science.’”
**The Expanse system**

The Expanse machine, built by Dell Technologies, will provide 5 petaflops of peak performance with top-class Dell EMC™ PowerEdge™ servers with AMD EPYC™ processors and NVIDIA® V100 Tensor Core GPUs. The system has been designed to provide ultra-high performance and data movement capabilities to fit the extreme diversity of applications at SDSC. Strande says Expanse will provide an increase in throughput by a factor of at least 2, relative to the center’s previous system Comet, while supporting an even larger and varied research community.

“Expanse’s accelerated compute nodes will provide a much-needed GPU capability to the user community, serving both well-established applications in areas such as molecular dynamics, as well as rapidly growing demand for resources to support machine learning and artificial intelligence,” he adds.

Strande says that server GPU acceleration was a required component of the system based on near 100% utilization of the server accelerators on the previous system, Comet. From molecular dynamics, neuroscience, materials science, protein structure analysis and phylogenetics, going the all-CPU route was not even a question.

“Our GPUs on Comet are chock-a-block full with jobs and we routinely reduce by half the amount of time that we can allocate to GPU proposals versus how much time reviewers recommend,” Strande says. “From application readiness efforts that are under way now for systems like Summit, and Perlmutter [two leading-edge national supercomputers], it’s clear that the demand is there for large GPU-based systems, and the growth in machine learning and AI will only increase this demand.”

Strande notes that systems like Expanse, though modest in comparison to some national GPU-based systems, provide a vital onramp for NSF users and those who are planning for scale-up on these large systems.

“There is a strong demand for GPUs as evidenced by our Comet user community and the general lack of GPU resources available to the NSF research community,” he adds. “We serve a diverse workload that includes applications from many domains that require GPUs. And in our view, it’s important that we help our users move towards architectures like GPUs, which have the potential for substantial price/performance benefits and represent an important pathway for users who are moving to exascale.”

SDSC’s GPU wisdom has been fueled by experiences handling mixed workloads at scale on Comet, where most of the GPU cycles were allocated to single GPU jobs, thus having more in a server is advantageous. By and large, most of the GPU applications are not CPU-bound, and SDSC found that in most cases the 2:4 ratio of CPU to GPU is about right. Expanse will use PowerEdge C4140 servers with NVLINK so users that run on multiple GPUs will see a nice performance gain over what they had in Comet (which will remain operational through 2020).
Strande says they certainly would like to have more GPUs, but again, in terms of capacity and utilization, the balance they have in Expanse of 56x two-socket CPU nodes and 4x 4-way GPU nodes per scalable unit (essentially a rack) is ideal. This is also a very good design point for the Mellanox HDR 100 interconnect, which provides a single HDR 100 connection down to the nodes, and a 3:1 oversubscription between scalable units. All of this means excellent latency and bandwidth with a single HDR 200 switch per scalable unit.

While GPUs are found on many top-performing supercomputers, it is only recently that AMD EPYC processors are coming to the forefront as a competitive choice. SDSC decided on EPYC after careful consideration of the workload and performance gains possible with the new generation of AMD processors.

“The choice of any given processor is highly dependent on the deployment schedule of a given system,” Strande explains. “What makes sense today, may not be the best choice in six months. Expanse will be deploying the 64c EPYC 7742, which will give us 128 cores/node. This is an excellent fit for the shared node jobs that represent a large fraction of the Expanse workload. Our initial benchmarks with the EPYC indicate that we will see at least a two-fold improvement in job throughput over what we have on Comet today, and that is at the core of giving the community a capacity system. Notwithstanding the focus on modest-scale jobs, it’s noteworthy that one scalable unit of Expanse contains over 7,000 cores in a fully connected HDR 100 network.”

IN JUST OVER 4 YEARS:
- 40,000+ Unique Users
- 1,200+ Publications
- ~2,000 Research, Education and startup allocations
- 400+ Institutions
- Scientific discoveries and breakthroughs

SDSC WORKLOAD IS COMPRIS ED OF FIVE MODALITIES:
- Traditional batch-scheduled single core and modest-scale computing jobs (one to a few hundred cores)
- High throughput workloads, which are supported via integration with the Open Science Grid
- Science gateways, which are now a ubiquitous way of accessing HPC
- Direct cloud bursting from the on-premises system via the scheduler
- A composable system feature that is best described as the integration of computing elements (e.g., some number of compute, GPU, large memory nodes) into scientific workflows that may include data acquisition and processing, machine learning, and simulation.

Expanse is a heterogeneous architecture designed for high performance, reliability, flexibility and productivity

**System Summary**
- 13 SDSC Scalable Compute Units (SSCU)
- 728 x 2s Standard Compute Nodes
- 93,184 Compute Cores
- 200 TB DDR4 Memory
- 52x 4-way GPU Nodes
- 208 V100/follow-on GPUs
- 4 Large Memory Nodes
- HDR 100 non-blocking Fabric
- 12 PB Lustre High Performance Storage
- 7 PB Ceph Object Storage
- 1.2 PB on-node NVMe
- Dell EMC PowerEdge
- Direct Liquid Cooled
ABOUT THE SAN DIEGO SUPERCOMPUTER CENTER

• SDSC is a leader in all aspects of advanced computation, including data integration and storage, performance modeling, data mining and predictive analytics, and software development.
• SDSC provides resources, services and expertise to the national research community, including academia, industry and government.
• SDSC supports hundreds of multidisciplinary programs spanning a wide variety of domains, from astrophysics and bioinformatics to environmental sciences and health IT.
• SDSC is a Dell Technologies HPC & AI Center of Excellence.

Scalable compute units

The scalable compute units are a unique feature of the Expanse machine. Each of these has 56 two-socket CPU nodes, 4 GPU nodes with 4 NVIDIA V100 Tensor Core GPUs each, and a 40-port 200 Gb/s HDR InfiniBand switch with 60 100 Gb/s links down to the nodes, and the remaining 10 200 Gb/s uplinks to the core.

The concept of the scalable compute units meshes well with the workload profiling efforts at SDSC based on the Comet system, also built by Dell Technologies. Strande predicts that 90 percent of workloads can be done at scale in a single unit since they are dense with high core counts and all the right interconnect network infrastructure is in place. The plentiful local NVMe for local I/O is fast and shatters through bottlenecks that have been problematic on large systems with parallel file systems. The Lustre storage system with HDR 200 further enhances I/O performance. All CPU nodes are liquid cooled, which ensures that the dense system reaches the highest levels of performance and reliability.

In the midst of balancing for workload diversity, SDSC also has other constraints: utilization and efficiency. The team behind Expanse is required to achieve 95 percent availability on the system with similar figures for job success. Comet excelled against these targets and Strande expects Expanse will be no different.

As Expanse gears up for full production, Strande says there is nothing more satisfying than putting a system on the floor. “I take joy in knowing that these systems are a vital element of the enterprise of science and research. You take pride in doing this kind of work and making these systems highly available.”

Working with Dell Technologies and NVIDIA

Strande says that having great partners like Dell Technologies and NVIDIA makes all of this possible, in part because the teams understand right-sizing system components to meet the needs of highly diverse workloads.

“We had an outstanding partnership with Dell and NVIDIA,” he says. “The process is highly accelerated and collaborative, and very quickly, you home in a partner that can support you in the technical and proposal work. We talked to multiple vendors, looked at their product roadmaps, their support, their track record, and of course, the price. We approach this from a best-value standpoint.”

Ultimately, Dell Technologies and its partners proved to have the right capabilities and technologies to deliver and support the Expanse system.

“A very competent group of people who really understand the workloads and share in the same design philosophy,” Strande says. “When the system is in production and problems arise — and every HPC system has some when you’re working at the bleeding edge — you need a vendor that’s going to jump on that with you and solve that problem. They know what it takes, what to do, and they’re going to be available. They are going to show up if you need a part, or if you have a tough technical problem on the systems or application side, they are going to be there for you.”