

Introduction

Founded in 2005, University of California, Merced (UC Merced) is the newest campus in the University of California system with a focus on educating and training a highly diverse and underserved student population. With more than 65% of undergraduate students identified as first-generation college students, UC Merced continues to build on its growing reputation of excellence and innovation.

UC Merced is still in the early stages of attaining initial core facilities, building the platform to empower research objectives while providing their faculty and their students the tools they need to be successful. The university has built the majority of its research IT environment (compute, network and storage) within the last ten years, and most of it from scratch, but with growth comes need for additional computing resources.

The computational faculty has been awarded various grants to pursue their research initiatives, but they only had access to one shared scientific computing cluster for all student and faculty research.



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According to UC Merced's Christine Isborn, undertaking the installation and integration of a new cluster initially seemed daunting, since the system administration support staff at UC Merced can be very busy at times with the many IT projects underway.

"While this cluster was a welcome addition to our research programs, we weren't sure how to get the most out of it from a scientific computing standpoint. Silicon Mechanics treated us like a partner, however, and as a result the integration and installation has been very smooth, and when we have questions about usage they are answered immediately."

Dr. Christine Isborn
Assistant Professor of Chemistry
and Chemical Biology
University of California, Merced

Challenge

UC Merced wants to be a known player in Scientific Computing across scientific disciplines, including Biology, Chemistry, Materials and Mechanical Engineering, Physics, and Applied Math. For example, the Chemistry department is made up of 12 faculty members, four of whom are computational scientists. This is relatively a large percentage of computational scientists compared to established Chemistry programs in the University of California system.

Strategically, UC Merced is striving for a higher percentage of computational scientists than what is considered normal. The reason for doing so feeds into a long term plan to turn scientific computing into an area that UC Merced is known for worldwide. One challenge, prior to receiving the RCG grant, was not in recruiting computational scientists to its program, but rather convincing them that UC Merced had the computational features to keep them there.

Each faculty member that gets hired at UC Merced receives startup funds, which could be used to build a small cluster that works for his or her initial

needs. However, historically these clusters only offered traditional CPU nodes where today's computational scientists need graphical processor units (GPUs) in order to create more dynamic visualizations and to create larger and longer scale simulations than are possible on clusters outfitted with CPU nodes.

"GPUs were originally optimized for massive parallelization for video games, but that parallelization can also be used to accelerate our scientific calculations," says Christine Isborn, UC Merced's Assistant Professor of Chemistry and Chemical Biology. "With GPU technology we can take our science in totally new directions, because it allows us to perform larger and more realistic calculations. In fact, GPUs can do more than make our scientific calculations speed up, they can help the university access new realms of science not accessible otherwise."

Prior to being awarded the RCG, most faculty at UC Merced did not have the necessary budget to purchase clusters outfitted with GPU nodes, which can cost in upwards of six figures. Federal funding for scientific computing and

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research universities has largely dried up in recent years, and like other universities, UC Merced was forced to scramble for funding and donations.

Solution

During the Fall of 2015, the team at UC Merced took action in the form of submitting for an annual award called the Research Cluster Grant, offered by Silicon Mechanics and its partners, Intel, NVIDIA, Mellanox, Supermicro, HGST, Micron, Seagate, Western Digital and Bright Computing. The RCG provides the awardee with a full HPC cluster valued over \$100,000, to be used by that institution at its own discretion so long as it is research based.

In April of 2016, UC Merced and another institution (University of New Orleans) were both awarded HPC clusters as a result of applying for the RCG program; both grants were largely based upon the deep and immediate needs expressed in each application, and decided upon by an established committee. By obtaining the RCG grant, UC Merced had curated exactly what it needed, a cluster outfitted with GPU nodes.

Results

Since implementing and integrating its new cluster, UC Merced's SC department has experienced the following benefits:

1. UC Merced can now perform simulations to compare two different forms of pyruvate kinase. One is a form that shows up in many forms of cancer and affects the metabolism of tumor cells. The new cluster has allowed us to extend the time of the simulation enough to begin to see structural

changes. Our previous simulations were not sufficiently long enough, and it was difficult, if not impossible to discern any structural changes.

2. UC Merced is now extending and increasing the size of ensembles of simple disordered polymers. The new cluster allows more of these smaller simulations to be run in parallel since it scales very well to use one simulation per GPU for up to four very efficient simulations per node. The applications for this sort of research are very broad, but the type of things that most people would be familiar with are neurodegenerative disorders where disordered proteins are commonly involved. Some common disorders that most people are familiar with: ALS, Parkinson's, and Alzheimer's.

3. UC Merced is using the cluster to perform molecular dynamics simulations of DNA binding to different ions. Its research team is now able to get to much longer time scales than with its other cluster resources (300 ns instead of 50 ns). With these longer time scales, the team saw that its previous calculations were not properly equilibrated, which gave incorrect results. The new cluster allows the team to properly equilibrate its system, and at the same time changed its interpretation of ion-DNA binding. This work has applications for using DNA, not just in a biological context, but also using DNA as a nano-material to develop biological sensors. This is done by controlling the spatial organization of biomolecules (such as DNA) on a surface and by better understanding DNA-ion-surface binding interactions.

4. The new cluster is also playing a central role in a new project using quantum mechanics to model how

aggregates of molecules interact with light, which will allow UC Merced to model larger-scale and more realistic systems. This research team plans to use these studies to engineer molecules for applications as electro-optic switches or new photovoltaic materials.

The RCG high-performance cluster awarded to UC Merced represents a big step forward for a growing university looking to be known for its computational science and scientific computing prowess. With additional computational power and GPU-enabled technology, UC Merced continues to transform its technology foundation while enabling future research and discovery opportunities. UC Merced is said to be "Built for the 21st Century" and Silicon Mechanics is honored to be part of this future for its faculty, current and future students.

HPC Cluster Solution Components

Intel Xeon E5-2600 processors
Mellanox InfiniBand EDR networking
NVIDIA Tesla K80 GPUs
Supermicro SuperServer
Silicon Mechanics design, integration and support

Research Cluster Grant Contributions

