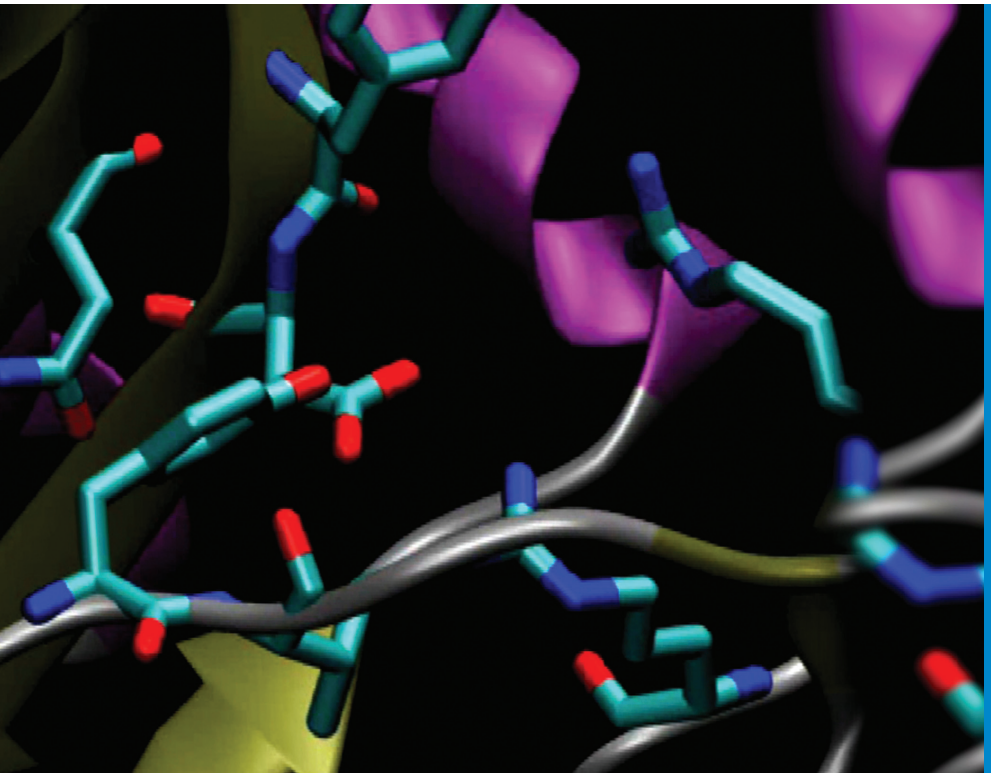
University of California Irvine gets 45% more research done with Dell and Intel HPC cluster

- HPC



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Ronald D. Hubbard,
Executive Director, GreenPlanet HPCC,
School of Physical Sciences,
University of California Irvine

Customer Profile

Company:	University of California Irvine
Industry:	Education
Country:	United States
Students:	34,000
Faculty:	2,685
Web:	www.UCIrvine.edu

Business Need

University of California Irvine (UC Irvine) School of Physical Sciences needed its own high-performance computing (HPC) cluster to provide its 27 research professors and their teams control over their own destiny. Previously researchers handed out their data to HPC centers for analysis and did not have 24x7 access to it.

Solution

The university worked with Dell and Intel to help design and build an in-house HPC solution using Dell™ PowerEdge™ servers with Intel® Xeon® processors, Dell PowerVault™ MD1000 direct attached storage arrays and QLogic TrueScale InfiniBand interconnect.

Benefits

- **45% more research done than with previous solutions**
- **33% increase in performance compared with previous solutions**
- **24x7 access to data for researchers**
- **10 federal grants won out of 11 grant applications**
- **28% energy savings**
- **23% space savings**

When Former Vice President Al Gore won the Nobel Peace Prize in 2007 for his work on climate change, he shared the prize with 34 researchers on the Intergovernmental Panel for Climate Change, 11 of whom do their research at the University of California Irvine (UC Irvine), School of Physical Sciences. Three other researchers have received the Nobel Prize during their tenure at UC Irvine: Frank Sherwood Rowland (Chemistry, 1995), Frederick Reines (Physics, 1995) and Irwin Rose (Chemistry, 2004).

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>
> *Douglas Tobias,*
> *Professor of Chemistry,*
> *University of California Irvine*

One of the 10 universities in the University of California system, UC Irvine prides itself on its distinguished history of scientific research.

Yet until a few years ago, UC Irvine did not have sufficient homegrown compute power to support its award-winning Nobel groups or its young and innovative researchers in such areas as atmospheric chemistry, bioinformatics, biopharmaceutical engineering and other disciplines that focus on chemistry and synthetic chemistry. Its researchers had to outsource their data to high-performance computing (HPC) labs such as the Fermi Lab in Chicago, the National Center for Atmospheric Research in Boulder, Colorado, the Stanford Linear Accelerator Center in Menlo Park, California and the San Diego Supercomputer Center.

"Our researchers were not in charge of their own destiny. They needed to be able to access their own data on an hourly basis, and they needed compute power that would speed up the pace of research," says Ronald D. Hubbard, executive director, GreenPlanet HPCC, School of Physical Sciences, UC Irvine. Hubbard was also recently named a 2010 laureate by the ComputerWorld Honors program for his work on a case study outlining collaboration between UC Irvine's dark particle physicists and Intel Corp.

Seeking partners in progress

Each of the large research groups at UC Irvine got together with Hubbard, and they decided that UC Irvine needed an HPC solution. "We put together a plan and we decided that the only way we could make it work was by having partners in progress, not just vendors," says Hubbard. "Dell and Intel rose to the challenge through their CEOs, Michael Dell and Craig Barrett, who committed themselves to high-performance computing at UC Irvine. They put us in a position where we could get their advanced tools and their advanced products—not necessarily off-the-shelf products—by opening their engineering and design-build processes to us and ultimately allowing us to do work that we couldn't have done without their help."

UC Irvine's HPC solution, GreenPlanet, started with 88 Dell PowerEdge 1950 servers and 14 PowerEdge 2950 servers with Intel Xeon processors. QLogic TrueScale InfiniBand interconnect, sourced through Dell, provided high thoughput, low latency connectivity among the nodes. Dell PowerVault MD1000 direct attached storage arrays delivered rack-dense, scalable storage.

Technology at Work

Services
Dell™ Hardware Customization Services
Intel® Cluster Ready Program

Hardware
Dell PowerEdge™ C6100 servers with Intel® Xeon® 5600 series processors
Dell PowerEdge C1100 servers with Intel Xeon 5500 and 5600 series processors
Dell PowerEdge R710, R610 and R410 servers with Intel Xeon 5500 and 5600 series processors
Dell PowerEdge 2950 and 1950 servers with Intel Xeon processors
Dell PowerVault™ MD1000 direct attached storage arrays
QLogic TrueScale InfiniBand interconnect

Tapping federal grants

With the infrastructure in place, federal money followed.

"Due to our activity in the science community with the National Science Foundation, the National Institutes of Health, the Department of Energy, the Department of Defense and NASA, we've applied for and received grants to expand GreenPlanet over these past 17 months from 102 nodes to 327 servers," says Hubbard. "We applied for 11 grants and got 10."

UC Irvine's federal grants span a wide spectrum of scientific activities. A $20 million grant for UC Irvine's Chemistry at the Space Time Limit (CASTL) project, will enable researchers to look at photographs of chemical reactions within cells for the very first time using high resolution video images. Other projects on the macro-end of the spectrum will gather data about the deepest novas in the universe.

"In between, we have really strong staples of atmospheric chemistry, coupled with synthetic organic chemistry, as well as pharmaceutical chemistry and a great deal of climate and weather modeling that takes place from the 30,000-mile level via satellite right down to the ground level on a minute-by-minute basis," says Hubbard.

33% increase in speed

The 327 servers in the expanded cluster include Dell PowerEdge R710, R610 and R410s servers with Intel Xeon 5500 and 5600 series processors. "Currently, we are procuring Dell PowerEdge C6100 and C1100 servers purpose-made by Dell with Intel Xeon 5600 series processors, Intel's newest and most advanced processors," says Hubbard.

With four two-socket server nodes in a 2U rack chassis, the PowerEdge C6100 is a hyper-scale-inspired building block for HPC environments and cloud builders.

"Through the efforts of Dell and Intel, we've been able to accelerate our activities plus we're seeing great energy savings and space savings in being able to do a greater amount of work in the same footprint," says Hubbard. "In fact, we're able to do a lot more work than we ever thought we could because of the advancements that Dell has made in their Cloud 6100 series servers. The Intel Xeon 5600 series processors have enabled us to work with a 33 percent increase in speed and a 45 percent increase in the amount of data that we can acquire and maintain. The partnership between Dell and Intel has definitely allowed us the opportunity to speed up our processes in the way that we deploy our software codes."

The Dell and Intel solution also saves 28 percent in energy consumption and 23 percent in space.

"Anytime a university like ours is looking for new partnerships, we're looking for a lot of ingredients. And what Dell has been able to bring through their partners are the roadmaps and the highways to do more dense and scalable research computing. Without that GreenPlanet would not be a reality, and without that GreenPlanet wouldn't be productive. And it's through the Dell process and the process of their partners that we've been able to be so successful in a very short period of time. GreenPlanet was designed to be an enabler of new discoveries. In order to make that design work, it takes a lot of people, a lot of process and a lot of production. Dell and Intel, more specifically, have been partners that have allowed all that to happen."

Simplifying acquisition and deployment

In addition to opening up its design and build processes to enable UC Irvine to obtain the advanced tools that it needed to do more science in less time, Dell worked with Intel to bring UC Irvine into Intel's Cluster Ready Program. Intel Cluster Ready certification includes comprehensive testing and integration work, enabling Dell HPC clusters with Intel Cluster Ready certification to simplify acquisition and deployment.

UC Irvine also took advantage of the Dell Hardware Customization service that integrates hardware, images, applications, peripherals and documents with systems as they're being built.

"With the integration that Dell does and getting the product preassembled and put into our cluster, we have become more efficient and proficient in the way we monitor and manage on a daily basis," says Hubbard. "GreenPlanet HPC is powered by Linux. We run multiple applications. We run very diverse software codes across 27 different professors and their research groups.

> "We study systems with hundreds of thousands of atoms and simulate their behavior. So, it's very important for us to have access to a large number of processors that have very fast interconnect. And the great thing about GreenPlanet is it satisfies those constraints for us."
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> *Rommie Amaro,*
> *Assistant Professor of Pharmaceutical Science and Computer Science,*
> *School of Physical Sciences,*
> *University of California Irvine*

And inside all these research groups are divergent codes that take weeks or hours to run. Through Dell's and Intel's expertise, we've been able to integrate all these into the cluster by using the Intel Cluster Ready Program and Dell Hardware Customization services. This has helped us to monitor and manage all these divergent activities on an open platform."

Faster cures for diseases

With the acceleration of science that UC Irvine is achieving with its GreenPlanet cluster, the result could be faster cures for diseases known as neuro degenerative diseases, such as ALS, Multiple Sclerosis, Alzheimer's, Parkinson's, Huntington's Disease, and cell degeneration, which are caused by the disturbed function of ion channel subunits or the proteins that regulate them.

Douglas Tobias, professor of chemistry at UC Irvine, is working on the computational chemistry that simulates molecular scale details of how proteins in voltage-gated ion channels open and close in response to changes in voltage. This is the basis of what's called the action potential, which is the electrical signal in muscles and nerves, and excitable tissues in general.

"When I started my research, I was very happy to be to be doing cutting-edge research by simulating approximately 800 atoms," says Tobias. "And now with GreenPlanet we're doing routinely a quarter of a million atoms and for two or three orders of magnitude longer in time. The type of system that we can study has been completely changed. We've gone from small molecules to large assemblies of macro-molecules. This opens up the landscape of the type of questions that you can ask. The more we can sample the underlying distribution or the dynamics, the more confident we can be in the results. And sometimes just running for a longer time lets you see things that you didn't see before, and couldn't have imagined seeing before. It's really transformed our research."

Developing new drugs

Rommie Amaro, assistant professor of pharmaceutical science and computer science, is studying a variety of infectious diseases. "In my lab we are using different computational simulations to try to understand how enzymes and biomolecules within these diseases behave and how we can come up with new drugs to target these specific enzymes," she says. "We study systems with hundreds of thousands of atoms and simulate their behavior. So, it's very important for us to have access to a large number of processors that have very fast interconnect. That allows us to get results much more quickly. And the great thing about GreenPlanet is it satisfies those constraints for us."

"We're so happy and so excited to have Dr. Rommie Amaro here, who is doing research at the leading edge of bio-synthetic research," says Hubbard. "We are very hopeful that those discoveries will lead to compounds and groups of compounds that will be converted into new medicines for new applications in the very near future."

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