For a research race potentially affecting tens of millions of lives, Pharmasset chooses the HP BladeSystem

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—Jim Anuth, Director of Information Technology, Pharmasset

HP customer case study:
energy and space efficiency

Industry:
healthcare

Objective

Deploy maximum computing power within tightening space, power, cooling, and administration-time requirements

Approach

Deploy HP ProLiant c-Class Server Blades in an HP BladeSystem c3000 enclosure

IT improvements

- Double the number of processor cores in less space than competitors
- Projected one-third fewer BTUs per hour than competitive solutions
- 50% reduction in time to value due to HP Insight Control management software

Business benefits

- Potential faster time to breakthrough by maximizing compute power in tight space
- $90,000 hardware cost avoidance through HP ProLiant quad-core, quad-processor architecture
- $90,000 in software licensing cost avoidance due to reduction in overall number of processors in the solution
- $5,000 in electrical work cost avoidance by being able to use 110V power instead of 220V

High stakes
The race is on: It's mind vs. matter.

"Matter" is represented in one of its hardiest and most dangerous forms: the virus. Specifically, this is a race to treat the devastating conditions caused by Human Immunodeficiency Virus (HIV), Hepatitis B (HBV), and Hepatitis C (HCV).

"Mind" is represented by researchers who are exploring and searching for novel classes of compounds to inhibit the functions of the natural proteins required for viral replication.

At stake in this race is the quality of the lives of more than 33 million people worldwide who are infected with HIV, 200 million infected with HCV and 360 million infected with HBV.[1]

[1] HIV carrier statistics: www.avert.org/worldstats.htm
Hepatitis B carrier statistics: http://features.us.reuters.com/wellbeing/news/B734D4EE-F5AE-11DC-AB07-925B7715.html
Hepatitis C carrier statistics: http://bmj.bmjjournals.com/cgi/content/full/328/7447/1031-a

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If researchers can find the right compound—one that inhibits the replication of any of these viruses—it could be used to treat viral infections and improve, extend, or even save those lives.

This race is underway at many locations. One of them is Princeton, New Jersey, at a company called Pharmasset, Inc. One of the many levels of research work taking place there happens not in a lab, but inside a number of high-powered silicon chips in the company's server room—on four server blades in an enclosure about the size of a small dormitory refrigerator.

How to thwart a deadly virus

Pharmasset's head of computational chemistry, Ralph Mosley, uses those server blades to perform molecular docking with the goal of identifying potential inhibitors of viral replication—a type of test that *could* be performed by Pharmasset's biologists in a real lab with pipettes and 96-well assay plates. But, by simulating the tests on a server, Mosley can run them much faster. This saves time and effort for the experimentalists by allowing them to focus on the compounds most likely to be effective inhibitors. Aside from docking existing compounds, Mosley can put virtual molecules together that look similar to components of DNA or RNA in ways that haven't occurred in nature yet. Either approach could lead to the good news that millions of people are hoping for.

"There are about 350,000 molecules in our database, all of which have to go into a binding cavity and a protein in our simulation," Mosley explains. "There are usually different conformations for each molecule being tested, if you will, in a binding cavity. So we need to be able to run up to between five to ten million simulations over 18 hours or so."

Mosley and other researchers then analyze the simulation results to search for promising leads. Those leads will be further explored by researchers in the company's actual physical labs.

It comes down to this

How fast can the simulations be run? And how fast can the servers and simulation software needed to run them be deployed? These are two critical factors in this race, and it fell to Jim Anuth, Director of Information Technology at Pharmasset, to come up with the most appropriate computing solution. Every day, Pharmasset's competitors are racing to find the right combination first.

"Other companies big and small are conducting this high throughput screening in computational chemistry," Mosley explains. "Based on how these tiny molecular fragments sit inside of a binding cavity, they can be connected together to make a completely novel drug."

If a drug is unique and can be patented, Anuth points out, "as it improves millions of lives, it could also be a billion-dollar product."

Which computing solution is right?

Pharmasset had just a 600-square foot server room and 45 people on staff in fall 2007 when Mosley joined. There were less than two racks of server space left, and the one-person IT staff was Jim Anuth. Another IT person has joined him on the team since.

About Pharmasset

Pharmasset (www.pharmasset.com) is a clinical-stage pharmaceutical company committed to discovering, developing, and commercializing new drugs to treat viral infections. In its search for a major pharmaceutical breakthrough, an IT infrastructure that delivers high compute density and low space, power, and cooling requirements give it a valuable edge.

"We needed the most computing horsepower we could fit into a limited space," Anuth remembers. "If we had to add power and cooling resources, we'd be looking at the six-figure expense of building a new server room. We didn't want to spend that money—or that time."

Pharmasset evaluated blade solutions from IBM, Dell, Sun, and HP. The proposed HP solution consisted of four HP ProLiant BL680c G5 Server Blades running Red Hat Enterprise Linux 4, each with four Quad-Core Intel® Xeon® E7340 series processors. They'd be housed in an HP BladeSystem c3000 enclosure.

"I evaluated the various solutions on a number of criteria, but in the end it all really came down to processor speed and density," Anuth says. "The HP BladeSystem met our speed, density, power, space and cooling requirements best." Pharmasset took possession of its HP BladeSystem in February 2008.

Immediate payback, saving $180,000

"I didn't see anyone else offering quad-core, quad-processor blades in such a small form-factor at the time," Anuth says. "The molecular modeling software we use is licensed per processor, not per core, so if we had chosen dual-core processors, we would have needed double the number of blades—an extra $90,000—and double the number of software licenses, another $90,000, to get the same performance. With the savings in software licensing alone, the HP solution paid for itself."

Fast deployment

Every hour until the system was up and processing was an expensive one, but Anuth liked what he discovered: "Deployment is intuitive and easy to master," he says. "The HP Virtual Connect Fibre Channel and Ethernet modules are integrated into the management console, and I was able to configure the Fibre Channel and gigabit Ethernet switches and the initial blade administration interface in about two hours. That's a huge benefit."

Reducing software deployment time by 50 percent

The company's software stack turned out to be challenging to install, optimize, and configure. "But the HP Insight Control Environment helped me work remotely," Anuth says. "Without it, I would have been living in the server room for probably about a month trying different permutations of software and configurations. Instead, I was able to complete it in two weeks—working virtually from my desk. The HP Insight Control Environment reduced deployment time by 50 percent. That's a huge HP advantage."

Saving power, cooling—and time
Two other advantages delivered additional savings. "The HP BladeSystem c3000 enclosure emits about a third fewer BTUs per hour than the other solutions I evaluated," Anuth comments.

The HP enclosure also enables Pharmasset to use an existing 110V power outlet. "By not having to put in a 220V circuit, we avoided $5,000 in additional electrical work," Anuth notes. "And most importantly, we saved time."

The "wow" factor
Research has begun, and Mosley is pleased with the speed of calculations: "When I speak with our software vendors or colleagues in our industry about the kind of throughput and compute density we're getting with the HP BladeSystem, you can almost see them salivate. They say they should move up to a system like that."

Anuth is pleased with the ease of management. "We have the equivalent of 64 1U pizza-box type servers in this one very small enclosure, which is so easily managed," he sums up. "I knew I was getting that when I did my research. But to actually sit down—virtually—in front of the HP BladeSystem and be able to get everything configured so quickly—that was a pleasant surprise."

"In all of this, CDW has been an invaluable resource to Pharmasset," adds Anuth. "Our account manager and his support team assisted in verifying our planned configuration and worked with us to ensure that we were able to stay within our project budget."

As you read this, the HP BladeSystem at Pharmasset is likely to be busy processing. The race is on. And if Jim Anuth, Ralph Mosley, and the rest of the team have their way, they'll turn mind vs. matter into mind over matter. The real winners will be millions of people whose lives are potentially improved or saved. And if that happens, it's likely those affected will have no idea that the key discovery began in a server enclosure the size of a small dormitory refrigerator, running quietly and coolly in a server room in Princeton, New Jersey.

Solution at a glance

Hardware
4 HP ProLiant BL680c G5 Server Blades each with four Quad-Core Intel Xeon E7340 series processors

1 HP BladeSystem c3000 enclosure

HP 4Gb Virtual Connect Fibre Channel Module

HP 1/10Gb Virtual Connect Ethernet Module

Software
HP Insight Control Environment (ICE) for BladeSystem

Schrödinger Suite

Accelrys Discovery Studio

Accelrys SciTegic Pipeline Pilot

Operating system
Red Hat Enterprise Linux 4

HP Services
HP Technology Services

Partner
CDW

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4AA2-0757ENW, July 2008