Astellas Pharma: New capabilities made possible by IBM BladeCenter accelerate discovery of high-quality drugs

Overview

- ***Business Challenge***
  Located in Japan, Astellas Pharma, Inc. (Astellas) needed to find a way to improve the speed of drug development. In the past ten years, parameters set by governing bodies have become stricter, and chemical compounds for testing have increased more than 1,000 percent. Astellas sought a research solution that would help it cut development costs, speed time to market and help meet energy efficiency goals.
- ***Solution***
  By implementing a high-performance computing cluster to support the drug discovery process, Astellas can streamline drug simulations and obtain more accurate results. Drug discovery applications now quickly process complex calculations and simulations to forecast a better selection of candidate compounds to be lab synthesized and tested.
- ***Key Benefits***
  - *Reduces calculation and drug simulation time by 90 percent*
  - *Contributes to reduced carbon footprint and reduced power consumption/cooling*

With a rich product portfolio combining a broad product range and sales scale, Astellas Pharma, Inc. is dynamically expanding its business in the global pharmaceuticals market. The company has discovered a large number of useful, reliable and highly competitive drugs. In addition to a sales system with global reach, its investment in a research and development system directed toward the discovery of valuable new drugs helps advance Astellas beyond its leading position in Japan and towards its goal of being a global top tier pharmaceutical company.

> *"With the IBM cluster technology, drug simulation time has greatly improved and that saves both precious energy and time for our researchers."*
>
> – Masaya Orita, PhD, research fellow, Astellas Pharma, Inc.

Business Benefits

- Reduces calculation and drug simulation time by 90 percent
- Contributes to reduced carbon footprint and reduced power consumption/cooling
- Helps eliminate bottlenecks in drug discovery research by enabling faster screening of compounds
- Enables a high degree of scalability to accommodate accelerating computing demands due to more sophisticated modeling techniques and an increasing number of candidate compounds

The Lead Chemical Research Group in the Chemical Research Laboratory, Miyukigaoka Center in Tsukuba, Ibaraki Prefecture, takes on the role of drug discovery research for Astellas Pharma. A high performance computing (HPC) cluster system, based on the IBM BladeCenter,® was built by this research group in order to rapidly and efficiently conduct drug discovery based on computational methods, in a reliable and stable environment. Simultaneous to playing a major role in eliminating bottlenecks in drug discovery research, the new cluster system made a major contribution in improving the motivation of the researchers.

Advances sought in drug discovery research

With the April 1, 2005 merger of Yamanouchi Pharmaceutical Co., Ltd. and Fujisawa Pharmaceutical Co., Ltd., the newly formed Astellas Pharma, Inc. took its first step as a global pharmaceutical company. As described in its business philosophy, new challenges continue daily in order to "contribute to the health of the world's people with advanced, reliable drugs." The company's aim is to achieve competitive dominance by providing high-value-added products to the world.

The company has positioned the Chemical Research Laboratory as the principal base of drug discovery research. The Lead Chemical Research Group is responsible for the upstream processes of new drug discovery and production processes and the goal of its research is the discovery of leading compounds optimal for becoming new drugs.

Masaya Orita, research fellow and lead researcher, Lead Chemical Research Group, explains that the environment enveloping today's pharmaceuticals market is changing drastically and is similar to the situation supporting drug discovery research: "Drug discovery research requires enormous expenditures. Consequently, an important issue becomes how to conduct this research efficiently. However, the environment has changed greatly compared to 10 to 20 years ago. There has been a dramatic increase in the number of parameters that must be considered, such as the efficacy and safety, and the pharmacokinetics of drugs referred to as absorption, distribution, metabolism and excretion (ADME). In addition, the number of compounds targeted for screening continues to increase. To perform highly accurate simulations and predictions while handling a large quantity of data, the power of high-performance computers is indispensable."

Shigeo Fujita, head of the Discovery Laboratory, Astellas Research Technology, Co., Ltd. continues, “There is high-throughput screening that uses an assay robot to empirically evaluate the compounds, as well as a mutually complementary method known as in-silico screening that performs virtual experiments on a computer. By applying this, the huge number of 15 million compounds becomes the subject of computation. Since about 2000, this research group has been studying systems suited to this huge computational scale.”

Accelerated increase in computation subjects leads to investment in large-scale systems

In this research group, prior to the introduction of a full-scale system, a cluster configuration was assembled in the company and two trials were conducted. In the first trial, Astellas’ Information Systems department built a cluster system from locations connecting multiple computers over a network. In the second trial, a test environment was prepared that combined commercial, low-cost computers and the cluster system.

“At the time, a large-scale investment still could not be made, and we did not go beyond the realm of trials,” reflects Fujita. “In other words, this was practice for an actual environment. Nevertheless, acceptable performance emerged, and the software we used was found to operate without any problems in the cluster system.”

In the next step – a full-scale application stage – an HPC cluster system was built based on the IBM eServer™ xSeries® 335 in 2003. Three years later, in 2006, plans were being made to enhance the system. This was not because of concerns about problems that the system had already reached its limit, nor had there been any issues with it. But by looking at the amount of data handled, which would continue to increase in the future, the decision was that sooner or later a larger scale system would be essential.

Solution Components

Hardware

- IBM BladeCenter HS20
- IBM eServer xSeries 335
- IBM eServer xSeries 336
- IBM eServer xSeries 346
- IBM eServer xSeries 206m
- IBM EXP400

Transformation at a glance

To bring new products to market faster in a highly competitive global pharmaceuticals market, Japan-based Astellas Pharma, Inc. built a high-performance computing (HPC) cluster based on IBM BladeCenter technology to support the critical drug discovery process. The new infrastructure helps Astellas work smarter and more efficiently by producing more accurate drug simulation results faster than was previously possible, thereby enabling Astellas researchers to quickly narrow the field of candidate compounds that may result in new drugs. In addition, the new computing solution has a much lower environmental footprint than older systems.

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– Masaya Orita

"The IBM eServer xSeries 335 demonstrated the expected performance," states Fujita. "But the number of available compounds and the structural analysis results of publicly announced target proteins are increasing annually and at an accelerated rate. In addition, new screening methodologies requiring more computations will also appear. In the future, faster computational speeds will clearly be demanded."

Thus, the research group that received IBM's proposal decided on the IBM BladeCenter as the basis of a new HPC cluster system to handle large-scale computation jobs.

Superior performance, energy efficiency and high reliability

The research group, which already had experience with the IBM eServer xSeries 335 and gave a positive evaluation to the IBM design concepts, did not hesitate to introduce the IBM BladeCenter.

"While in the trial phase, we faced many troubles which caused us to focus solely on operating the machines," explains Orita. "But after the introduction of the IBM eServer xSeries 335, we could concentrate on the research because of the high stability of the system. We were confident that everything would be fine even at a larger scale."

Fujita adds, "Surprisingly, there were no problems and troubleshooting was not necessary. The burden on the user was minimal, and the experience was truly pleasant. This high reliability provided a sense of security and confidence in the system."

In addition, an important element in the selection of the IBM BladeCenter was the energy efficiency. It was important to effectively use to the utmost, the installation space and the capacity of the air conditioning equipment. Another requirement was the pursuit of low power as the number of CPUs continued to increase. Even under these stringent conditions, the ability to conserve space and achieve high energy efficiency without sacrificing superior performance and stability was the decisive factor in selecting blade servers. In practice, this large-scale cluster configuration is compactly mounted in two 42U racks that include a login server and a file server. A feasibility study conducted at IBM clearly demonstrated the ability to achieve the target energy efficiency and performance. Naturally, reaching this stage necessitated a close relationship with IBM.

"What is the optimal configuration corresponding to the type and the scale of the computation? For the parts that we could not solve through our own efforts, we received comprehensive support with a broad perspective from the disk porting method and the disk capacity, the CPU estimates, the amount of heat generated, and the equipment space taken up by the operation," says Fujita.

Looking to the future, and strengthening the research foundation as the source of competitive strength

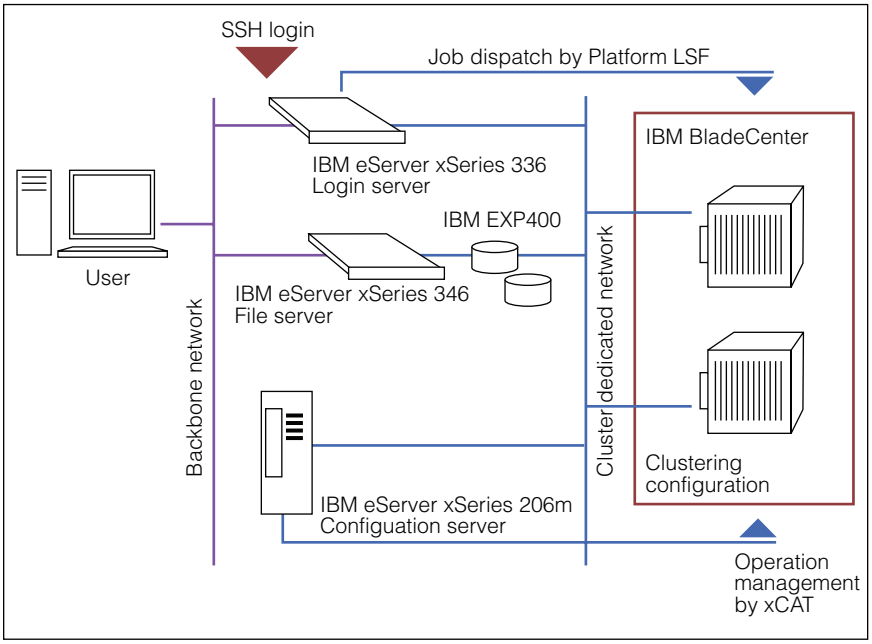
Operations began in December 2006. The most closely watched effect was probably the computational performance. By achieving eight to ten times the conventional speeds, what used to take one year now takes only one month. "Now we can do what we could not do in the past. This change broadens the range of possibilities immeasurably."

"We demonstrated this feature in the drug discovery project and could play the game in the true sense. The motivation of the researchers is definitely improving," notes Orita.

About Astellas Pharma: A system for growth

Astellas Pharma, Inc. continues to grow as a global top-tier, R&D-oriented pharmaceutical company originating in Japan. The company was established on April 1, 2005 with the merger of Yamanouchi Pharmaceutical Co., Ltd. and Fujisawa Pharmaceutical Co., Ltd. Astellas has developed a seamless system from research and development to sales, and helps to discover leading pharmaceuticals with superior utility and reliability. In drug discovery research, importance is placed on the six fields of urology; inflammation and immunity, including transplants; diabetes; central nervous system pain; infectious disease (viruses); and cancer.

System overview



In addition, Mr. Fujita is looking to IBM to fill a future role that goes beyond the ordinary relationship between an IT vendor and a customer. “Soon the era requiring 100 to 1,000 times today’s computational power will probably be here. To invest in the technology for that time, careful preparation is important. Scenarios are created, and the technical and environmental preparations are made and will be performed as soon as the time comes.”

For more information

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