CUSTOMER CASE STUDY

> “We seek to develop breakthrough drugs by integrating the accumulated drug discovery research outcomes of academia with those of pharmaceutical companies derived from the analytical simulation on cloud.”

Tatsuhiko Kodama
Professor, RCAST,
The University of Tokyo

Cloud service enables ‘in Silico’ drug discovery.

At a glance

Country: Japan
Industry: Healthcare
Founded: 1987
Employees: 304 faculty members and 84 students (as of March 1st, 2014)
Website: www.rcast.u-tokyo.ac.jp/en/

Challenge

Pharmaceutical companies and research institutes around the world are eager to harness cutting-edge science and technology in their quest for new drugs.

Solution

The University of Tokyo has its own supercomputer and high-performance computing (HPC) cloud environment and decided to use Fujitsu’s cloud service for analytical simulations.

Benefit

- Large-scale computing environment unconstrained by the power-consumption restrictions within the university campus
- Scalability of the cloud means future needs can be met by simply adding computing resources as research expands

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Customer

At the Research Center for Advanced Science and Technology, the University of Tokyo (RCAST) is pursuing interdisciplinary research covering key domains: information, biology, environment, material, universal-design and society. A sixth domain is biochemical medicine, and RCAST is trying to understand the mechanisms of diseases and pursuing R&D into new drugs.

Products and services

- FUJITSU Technical Computing Solution TC Cloud

Challenge

At the heart of traditional approaches to pharmaceutical R&D is the search for molecules with a desired effect from among those existing in nature. The current approaches are to discover potential drug candidates by screening existing compounds against target characteristics and to design new molecular combinations based on knowledge of physiology and molecular biology. Pharmaceutical companies and research institutes around the world are eager to harness cutting-edge science and technology in their quest for new drugs. Regardless of whether the approach is drug discovery or drug design, in practice, scientists select candidates that they think may have the desired effect from a knowledge base and modify their substructure to enhance their efficacy. Since the number of molecules in the knowledge base is limited, they are running out of possibilities.

The answer is to create new, previously unknown chemical compounds. Whereas the current knowledge base covers some 20 million (2x107) molecules, there are estimated to be as many as 1,020 molecules theoretically synthesizable. This opens up new possibilities in the quest for new drugs.

The relationship between a key and a keyhole is often used to explain metaphorically the efficacy of a drug. For example, at the time of the year when hay fever is rife in Japan, there are often TV commercials for sinus medicines that block the molecules that causes the allergy. Here, the key is the drug, and the keyhole is the specific section of a protein that triggers the allergy symptoms. Drug discovery involves finding a key that exactly fits the keyhole. Within silico drug discovery (the use of computer simulations to identify small molecule and other potential therapeutic drug candidates) drug candidates are screened by simulation based on 3D modeling of proteins.

Simulation is also used to home in on highly efficacious molecules from among the numerous candidates that have been identified. Experiments are unnecessary because the entire process is computerized.

By dispensing with actual synthesis of a molecule or testing in vitro or in vivo, this approach accelerates drug discovery and cuts costs. Since the performance of CPUs and other hardware is improving all the time, computer simulation allows testing of an increasing number of new molecules more rapidly at progressively lower cost.

Solution

RCAST's ambitious silico drug discovery initiatives are supported by Fujitsu's cloud service for analytical simulations, the FUJITSU Technical Computing Solution TC Cloud. With over 10,000 CPU cores and general-purpose computing on graphics processing units (GPGPU - technology that employs special processors originally used in graphic processing for general computational applications other than graphics processing) delivering theoretical peak computing performance of over 230 teraflops (a trillion floating-point operations per second) and 250 teraflops, respectively, TC Cloud offers performance comparable to that of a supercomputer.

Benefit

RCAST is leveraging TC Cloud's overwhelming computing power to speed the creation of promising new molecules for drug discovery. With TC Cloud, RCAST benefits from a large-scale computing environment unconstrained by the power-consumption restrictions within the university campus. The scalability of the cloud means future needs can be met by simply adding computing resources as research expands.

Going forward, RCAST is eager to conduct joint research with pharmaceutical companies and other private-sector enterprises. With TC Cloud on track to be the leading platform for drug discovery in Japan, a bright future beckons. That is why the University of Tokyo, which has its own supercomputer and high-performance computing (HPC) cloud environment, decided to use Fujitsu's cloud service for analytical simulations. This commercial HPC cloud service is available throughout industry, government and academia and therefore enables collaboration on simulations of candidate drug compounds.

TC Cloud opens the door to the development of new drugs outside the scope of traditional experiment-based approaches. Fujitsu ICT is working for the wellbeing of people worldwide.

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Phone: +81-3-6252-2220