Success Story

SGI® Origin® 3800 Supercomputer at SARA

A Crucial Component in Specialized Scientific Research

Computer simulations play an enormous role in the Dutch scientific world. Using complex calculations that require extensive computing power, a wide variety of academic disciplines work to gain greater insight into scientific, technical, and medical processes. These can include, for example, the effect of ocean currents on ships or offshore drilling platforms, instances for which every aspect of fuel consumption and hull optimization is accounted. Other scientific research concentrates on such issues as the analysis of the growth process of human bone tissue. By creating extensive bone simulations, scientists can test varying stresses on bone tissue, making the growth process more predictable. Studies of this kind require huge computing and storage capabilities, a stable management environment, and a user-friendly programming environment. For this fundamental, applied research, scientists make use of a centrally managed national supercomputer.

About a year ago, a new SGI® supercomputer was installed at SARA Computing and Networking Services (the Amsterdam Academic Computing Center). The supercomputer consists of two SGI Origin 3800 servers using a total of 1,024 processors, making it one of the most powerful computers in Europe. Its powerful performance (1 TFLOPS), massive memory (1TB), and storage capacity (10TB) have earned it the fitting name of TERAS, the Greek word for 'monster'. It's an especially impressive machine, with peak performance numbers about 100 times that of its predecessor.

Selection Requirements

In the Netherlands, the National Computing Facilities Foundation (NCF) —part of the Netherlands Organization for Scientific Research (NWO)—is responsible for the selection, acquisition, and use of the national supercomputer. Expansion of the computer's capacity is considered in conjunction with the ongoing development of scientific study. To keep the research at an internationally competitive level, and to meet the growing need for increased computing power, the NWO finances adaptations and any necessary revamping of the system. NCF's requirements generally involve computing power, speed, and storage capacity. This inevitably calls attention to price/performance ratios and the ability to allow for further expansion in the future.

Regarding the selection process, Bert van Corler, advisor at SARA's High-Performance Computing Division, says, "NCF carries the greatest weight when it comes to the selection process. When it comes to management and use, SARA is the responsible body. They emphasize issues such as accessibility, adaptability of existing programming, and demands on storage and software."

Benchmark
Following a primary selection process, a shortlist of suppliers was drawn up to perform a benchmark study. This involved efficiency tests and a throughput and interactive test based on performance measurements of the processors and internal networks. The evaluators also carried out concrete end-user programs and examined how the machines responded to a high degree of simultaneous use. The tests showed that SGI Origin 3800 provided the best performance.

According to Bert van Corler, "In terms of user programs, the input of existing code, and the throughput test—which consisted of a mix of user programs—SGI was the overall winner and came out on top. What's more, the SGI systems were attractively priced." In addition to the technical advantages, SARA was already managing a number of different SGI machines for other organizations, including the CAVE virtual reality facility and the UNITE system, which is an SGI® Origin® 2000 series system with 128 processors used by the University of Twente and the Technical University in Eindhoven. As a result, SARA already had experience with shared-memory programming and the various associated management tasks. SGI is also renowned for its development of solutions with highly demanding environments, such as scientific research.

TERAS has 1,024 MIPS® processors, each with a computing power of 1 GFLOPS, and 1GB of memory. The computer's total data processing capacity is 1 TFLOPS with an internal memory of 1TB. The system has access to 10TB of disk space and more than 120TB of near-line storage.

TERAS
"The SGI Origin 3800 machines are much more than new computers with more processing power and capacity," says Bert van Corler of SARA. "The architecture is structurally different than our last supercomputer, which was based on vector computing. SGI, on the other hand, uses parallel computing. Our old computer—a Cray C90—derived its power from vector processing, in which calculations are based on data that undergo the same arithmetic operations. TERAS is a massive parallel system, which derives its total capacity from many interconnected processors." TERAS is divided into partitions with the SGI cache-coherent nonuniform memory access (SGI® NUMA) architecture, which uses a single operating system so the user sees a single memory.

Transition
To have operations continue as smoothly as possible during the transition to the TERAS system, SARA chose to put two SGI Origin 2000 series machines into temporary use. The first SGI system—which has 32 processors—was installed in April of 2000. This machine was used chiefly for training, testing, and conversions. At a later stage, a second SGI Origin 2000 series system was installed. This one used 128 processors and took over some of the supercomputer's tasks until TERAS was installed.

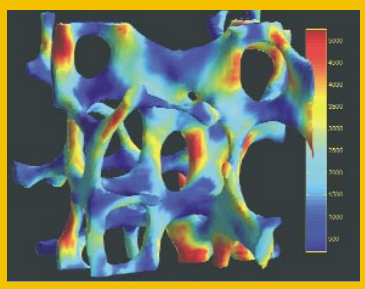
"The provisional Origin systems were largely meant to help end users get used to the new architecture and software environment," says Vincent den Elzen, TERAS project leader for SARA. "In this way, SARA could use the availability of SGI machines to expand on their knowledge and expertise. It also helped them to meet a variety of parameters, including the introduction of new software and the adaptation of storage capacity. As an example, the existing StorageTek tape robot had to be adapted and a temporary file server was installed in order to convert 11 terabytes of user files and then make them accessible from both the SGI and Cray systems. The SARA people were able to consult SGI professionals every step of the way and work as team."

Users
When it came to the computer's actual installation, the advantages quickly became evident to the users. "The new machine's peak performance is more than 85 times greater than the old one," says Bert van Corler. "As a result, we can make much greater demands on it. And, because the computer can handle much heavier commands, it can refine problems to a much greater degree. Not only does it handle more complex calculations, it does its work much faster, too. More complex and detailed simulations also translate into more reliable results, thereby enhancing the quality of the research."

Nevertheless, the SGI supercomputer's new architecture does require adaptation and effort on the part of the users. "The transition from vector to parallel computing will require TERAS users to adapt or parallelize their code and convert their data and software," says van Corler. "Only then can they make the best possible use of this new system."

Information Program
SARA drew up an information program to ensure that its users were kept up to date of all changes. Throughout 2000, SARA put together extensive Web documentation and a training course. It did this in cooperation with SGI and NCF to give future TERAS users a detailed view of the new possibilities and applications. To accelerate the acceptance process, users were given free access to the temporary SGI Origin 2000 series setup. Furthermore, SGI and SARA took extensive measures to guarantee users continuous access to their files. Of course, users were always able to call upon individual support for SARA whenever necessary, and SGI and SARA actively approached users to examine their problems in detail and provide advice and assistance with software porting, parallelization, and data conversion. With the help of some solid preparation, the ultimate transition to TERAS went according to plan, and the Dutch scientific community can now make full use of the supercomputer.

Simulations
A number of projects using TERAS's computing power are already under way. These include the determination of stress distribution in bone tissue and large-scale, quantum-chemical calculations of electron structures. At Erasmus University in Rotterdam, TERAS is being used in broad-span simulations in which entire bones are being worked into computer models. Research at the university's Orthopaedic Research Laboratory focuses on the analysis of bone tissue, as it is responsible for bone growth. The lab creates representations of bones using CT scans, after which it simulates bone growth and adaptation.



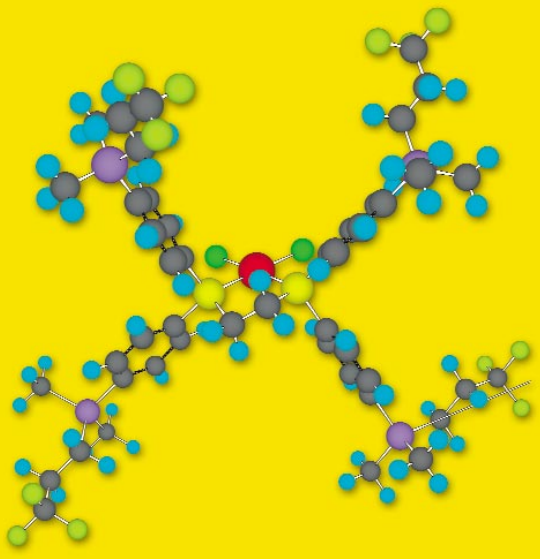
A piece of spongy bone taken from the vertebra of an 80-year-old woman, post mortem. The tissue deformation (expressed in microstrain) is reflected on a scale of up to 5,000 microstrain. Compression of the vertebra is plus or minus three times the body weight, and occurs regularly during the course of a normal day—with light lifting, for instance. These deformations were calculated using a program specially designed for this purpose, running on an NCF supercomputer.

"Before the SGI Origin 3800 system went into service, we worked mainly with simulations of small pieces of bone, which we analyzed using powerful PCs," says Harrie Weinans, PhD at Erasmus Orthopaedic Research Laboratory. "Now, with SGI Origin 3800, we can perform large-scale simulations in which we can analyze the stress distribution of entire bones."

In the Theoretical Chemistry of Utrecht University, Joop van Lenthe, senior lecturer, and collaborators perform painstaking complicated calculations on molecular structures of varying sizes. With the help of TERAS, the group has a great deal of processor power at its disposal, and the combined memory of the processors in use provides a capacity of hundreds of gigabytes. Now larger and more realistic molecules can be simulated in an acceptable time. This allows scientists to set ambitious objectives in their application of quantum chemistry, far beyond the relatively limited scope of the past. These are just two examples of the many areas of study for which TERAS's computing power is being used.

The Future

By choosing the SGI Origin 3800 supercomputer, the Dutch scientific world can now avail itself of one of the most powerful computers in Europe. To meet the ever growing demands of scientific research in the future, the supercomputer's expandability is equally significant. The SGI machine's scalable and modular construction allows for every eventuality, not only in terms of processing power (by installing more powerful processors) but also for flexibility, management, and maintenance.



A molecular model of a Perfluoralkyl-silyl-Ni(II) phosphine complex. It is expected that this molecule will act as a catalyst, which will either enable or facilitate a variety of chemical reactions.
From: A.C.A. de Wolf, Ph.D. thesis (Utrecht, April 25, 2002)

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