Chapter 9. Center for Computational Materials Science

Head : Prof. Y. KAWAZOE

Chief (Technician): K. ICHINOSEKI, 2 Technicians, 9 Part-time Employees

1. Organizational Structure

Since fiscal 2003, the Faculty has appointed the Kawazoe Laboratory as the department in charge of the Computational Materials Science Center to ensure highly integrated and consistent operations. Conventionally, the Laboratory has been positively involved in the Center's operation through activities such as hardware selection when introducing the supercomputer and equipment renewals, as well as monthly meetings with hardware and software suppliers. In addition, it has played an essential role in supporting and leading staffers at the Center who participate in and present research papers at academic conferences and workshops held domestically and internationally, as well as computer-related learning sessions aimed at brushing up relevant knowledge and skills. Regarding hardware sourcing, efforts were made to ensure that equipment supplied to the Center should be allotted as far as possible to research projects involving the Kawazoe Laboratory, to reinforce the facilities with constantly-updated equipment and to create opportunities for researchers to experience and learn the latest technologies.

An all-electron mixed-basis method program (TOMBO: TOhoku Mixed-Basis Orbital *ab initio* program), introduced to enable the Center's supercomputer to run at the maximum performance, has achieved as high as 70% of the performance rating given in the catalog specifications, improving the overall average to nearly 30% as well. In addition, joint efforts between suppliers and the Center's technical staffers have constantly improved the performance of the supercomputer, lifting its operating capacity beyond 90%. Recent demands for computing have shown remarkable growth, and working toward the establishment of a larger-scale computing environment to exceed the existing supercomputer installation, a trial project team has already been formed by the Institute representing the Super SINET Nanotechnology Research Panel and the National Academia Creation Program to test supercomputer connections, with our researcher K. Ichinoseki as a key person, jointly with the Institute for Solid State Physics of Tokyo University, the Institute for Molecular Science at the Okazaki National Institute and the Computing and Communications Center of Kyushu University, and an experimental optical computer network was accordingly set up. Interactions among supercomputers placed in geographically remote sites, along with super-large scale computational simulations, were tested in this unprecedented project, which it is an honor for the Institute to participate in as a first experiment.

Moreover, now that Special Coordination Funds for Promoting Science and Technology (SCF) have been approved as a result of medical-engineering collaboration, the Center will continue its positive involvement in new materials designs based upon first-principles computational simulations with supercomputers in order to pioneer innovative approaches to medical science through this project.

In accordance with the transition of national universities to independent administrative corporations in 2004, the Center was also off to a start with several studies in pursuit of an excellent organization. It is notable that there are three supercomputers operating on campus: in the Information Synergy Center, in the Institute for Fluid Science, and in our Institute, creating maximum strengths in each of these academic areas. Those three organizations are closely communicating with each other to discuss ways to utilize their hardware assets in the future.

Supercomputers are, and will continue to be, important items for national strategy. Taking advantage of their ability to offer efficient materials designs, they are essential items that can ensure Japan of an international presence in the field of materials manufacturing.

2.1 Usage During the Period

The numbers of users and jobs for services offered by the Center during the period are respectively 193 and 25,160.

Note that a summarized research report on using a supercomputing system was published in September 2004 (Volume 9 in the 2003 edition, including 79 original articles).

2.2 Overview of Super Computing System

The first supercomputing system in the Institute was introduced in 1994 and gave a remarkable performance, including assistance with generating approximately 350 original research papers during its seven-year service period ending in December 1999.

Progress in computer technology however has turned out to be amazing, and the performance level of our original supercomputer was brought down to the level of current top-end personal computers in the seventh year on a simple comparison. Thus it was replaced in January 2001, and the current supercomputing system offers features of high-speed large-scale computing that include 3-dimensional integration, large-scale sequence-involved calculations and fast Fourier transforms (FFT). Its huge memory capacity gives a performance equivalent to world-class high-end research facilities for materials design simulations after internal procedures for estimating and requisitioning the necessary budget. The configuration of the current system is shown in Fig. 1.

Our mainframe supercomputer is 40 times as fast in computing speed and 60 times as large in memory capacity as the first generation. The performance of the new machine, a Hitachi SR8000-G1/64, was ranked as 15th in the world in 2001, when it was deployed. In addition, the system includes an IBM RS/6000 S80 file server for users, a COMPAQ GS320 and SGI Onyx3400 as application servers and other equipment for use as the mail server, www server, and network management (firewall) machine, along with 30 workstations of various kinds.

Since the system was deployed, it has had an excellent track record, with success in determining the structure of the smallest basket-shaped stable silicon cluster containing a single metal atom by a first-principles computational simulation, and a quantitative explanation of the reason for the occurrence of Hund's Rule by accurately solving quantum mechanics equations using the Diffusion Quantum Monte Carlo method.

3.3 Setting up a Nanotechnology VPN

In order to set up a super large-scale nanotechnology computational simulation environment – "Super SINET" – through a network of supercomputers (VPN: Virtual Private Network) one of a very few in the world, four organizations – the Institute for Materials Research (SMR), the Institute for Solid State Physics of Tokyo University, the Institute for Molecular Science of the Okazaki National Institute and the Computing and Communications Center of Kyushu University – launched a collaborative project. All four participants were networked through a one-gigabyte connection on October 1, 2002 to start evaluating the communications efficiency, and then eight SR8000 nodes at SMR and six nodes of equivalent machines at the Institute for Molecular Science were exclusively used for experimental operations during the period from February to March in 2003. The purpose was to determine the most stable atomic structure of hydrogen clathrate hydrate through a demonstration experiment involving running two equivalent programs controlled in parallel with input parameters differentiated by an all-electron mixed-basis method program (TOMBO: TOhoku Mixed-Basis Orbital *ab initio* program). The Japan Advanced Institute of Science and Technology and Hiroshima University subsequently joined the project and were connected to the one-gigabyte network on October 1, 2004. At present, studies include visualizing the results of computational simulations. In addition, it has now been made possible to connect the Nanotechnology VPN to external networks by adopting firewalls. As a result, the network now has access to the computers at the Japan Atomic Energy Research Institute with the use of ITBL-based software, creating a larger parallel runtime environment.

Conceptual configuration for Nanotechnology VPN is shown in Fig. 2.

4. Visitors on Tour

During fiscal 2004, the Computational Materials Center hosted 165 Japanese and international visitors, including Professor Luo Jian-Hong from China's Zhejiang Medical University.

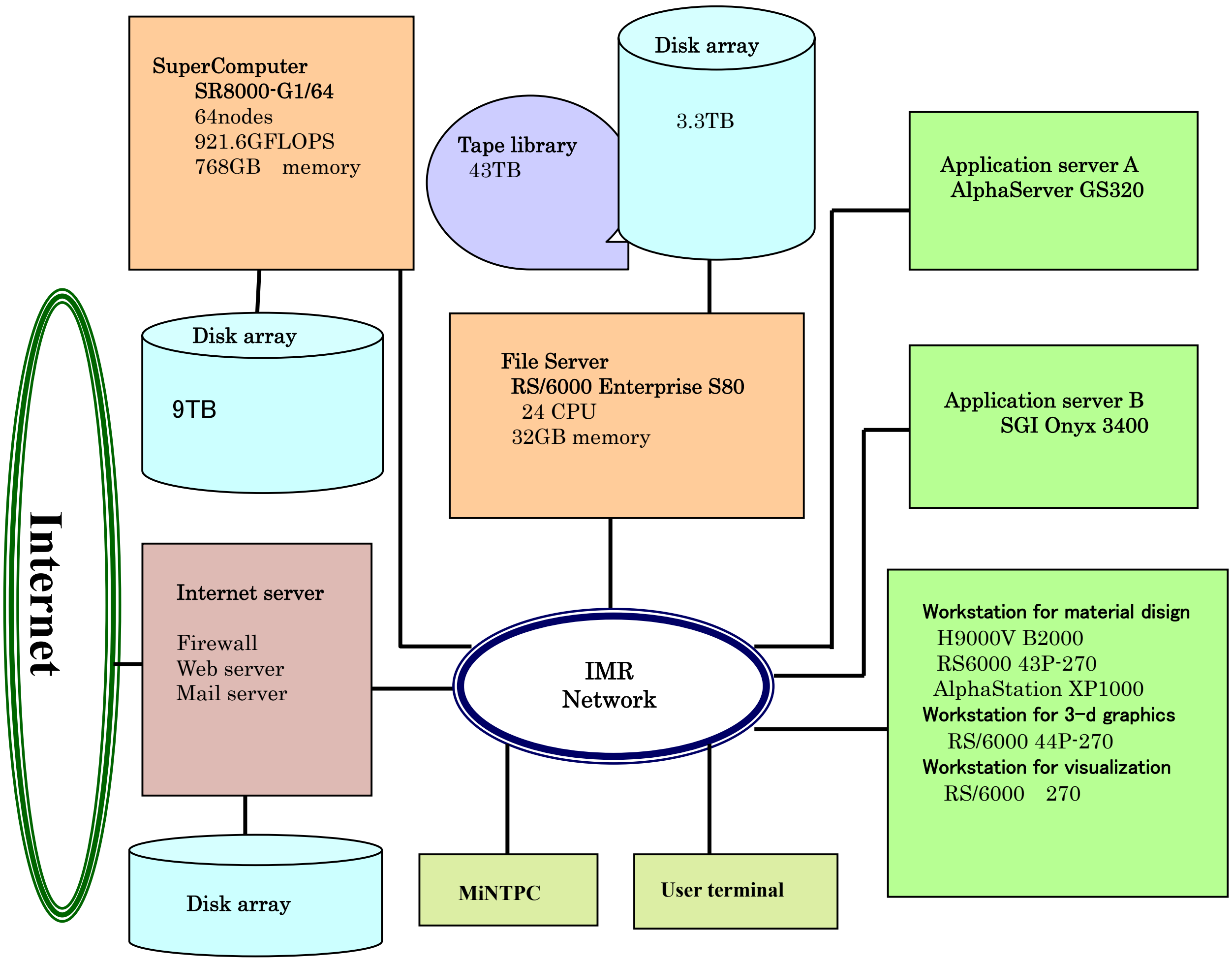

Fig. 1 The configuration of the current system

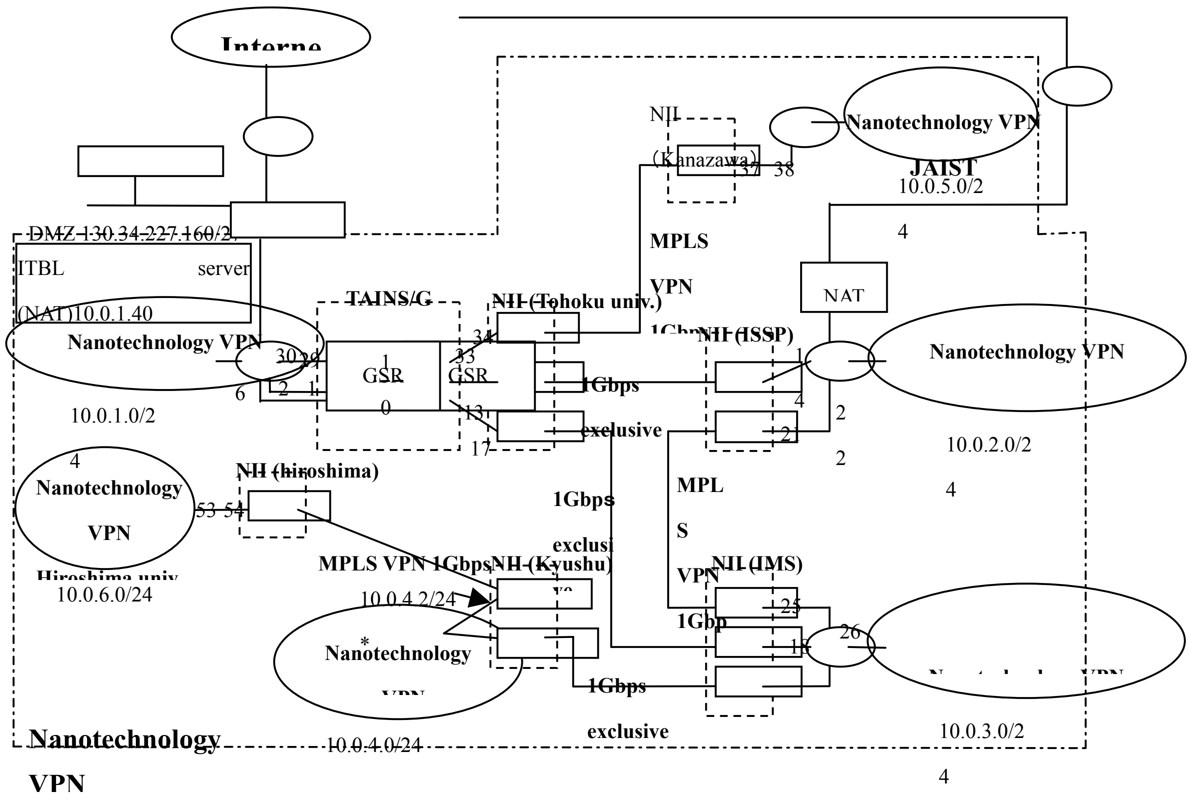

Fig. 2　Conceptual configuration for Nanotechnology VPN