NSRC's Outreach Experience

Chia-Ling Lee, National Supercomputing Research Centre, National University of Singapore, Republic of Singapore

ABSTRACT: The National Supercomputing Research Centre was established in 1993 to support both academic and industrial research. The Critical Success Factor for NSRC is encouraging Singapore organizations to find innovative use of the technology applied to their internal business processes and products. To reach out to industry, NSRC uses a number of approaches: training seminars and workshop are conducted where necessary, and company visits are often arranged for the trainer to meet industrial users. Such visits are critical since the users are more comfortable talking about their problems in a secured setting. Where possible, NSRC works with sister organizations in Singapore who have expertise in specific application areas. The expertise of Cray application analysts is heavily leveraged to complete some technology transfer projects.

Background of NSRC

The National Supercomputing Research Centre (NSRC) was established in 1993 as a government-funded Research Centre under the National University of Singapore (NUS). Although NSRC reports to NUS for administrative matters, the funding for NSRC comes from the National Science and Technology Board (NSTB), a statutory board set up to spearhead Research and Development efforts in Singapore.

The mission of NSRC is to enhance Singapore's global competitive position through effective use of high performance computing in research, manufacturing and services. With a 3-year budget of S\$42 million that was approved in 1995, NSRC has expanded significantly in scope and resources. Computing infrastructure now comprise:

- a Cray T94/2-128 installed in January 1996 with 1 GByte of memory, 1 GByte of solid-state device, about 60 GByte of disk and a peak performance of 3.6 GFlops,
- an IBM SP2 installed in June 1995 with 16 nodes, 2.75 GByte memory and 76 GByte of disk, and a total peak performance of 4.5 GFlops,
- and an NEC SX-3/11 installed in September 1994 with 256 MByte of memory, 24 GByte of disk and a peak performance of 1.37 GFlops.

In addition to the compute servers, NSRC also has over 20 workstations and an Visualization Laboratory with a 4-CPU SGI Onyx. The compute servers are connected by FDDI and ATM connections are been tested.

Currently, NSRC has a staff of 35, with 30 technical people, and about 1000 square metres of office space. The 1995 budget allows NSRC to expand to a head count of 38 technical staff. Bearing in mind that the application of high performance computing is new to Singapore, staff with high performance computing experience, particularly in an industrial setting, is scarce in Singapore. More than half of our staff have overseas degrees.

Technology Promotion

Training and Seminars

NSRC's general strategy is to provide and manage as a national resource, a top-tier supercomputing capability with a range of architecture and capacities. This national resource is targeted to stimulate the use of high performance computing in Research and Development (R&D) in Singapore. Therefore, in addition to powerful hardware, application software that are popularly used in R&D must also be made available.

As software is expensive, acquisition is based on the principle that only software that meets 90% of the requirement of industrial application are acquired. Companies with applications which are not met by our software suite may have to acquire their own license and load the software on NSRC machine(s).

A list of software packages available on NSRC machines is given below:

Structural Analysis:

MSC suite: Nastran, Abaqus, Dytran

- Marc
- CSA/Nastran (free trial)
- LS-DYNA3D (free trial)
- Ansys (free trial)
- PAM-suite: -Stamp, -Crash, (free trial) Plastic Injection Molding
- Moldflow
- C-Mold
- CMLogic

Computational Fluid Dynamics

- Fidap
- Fluent suite: Fluent, Fluent/UNS, Rampant, Nekton
- IcePak
- StarCD

Computational Chemistry

- Gaussian 94
- AMBER 4.1
- Unichem
- Cerius-2
- Discover
- Gromos

Chemical Process Simulation

- Speedup
- Aspen Plus
- Electronics Design Automation
- Hspice
- Medici, Tsupreme4
- Epic

Data Visualisation

- PV-Wave
- Khoros
- Iris Explorer Data Mining
- Intelligent Data Miner Front-ends
- MSC/PATRAN
- Hypermesh
- Hexar
- Ensight
- PAM-Station
- GeoMesh + TGrid

As the technology is new to Singapore organisations, training courses are organized on a regular basis. Courses are conducted by NSRC application analyst where possible. NSRC also works with the software vendor to organize training seminars that are half- to one-day long and workshops lasting 2 - 5 days. Examples of the latter include: FIDAP, IcePak, CMold, PAM-suite of software and up-computing workshops for Aspen Plus and Speedup. NSRC-organised seminars include Cray and SP2 user training, and Cray optimization training.

Seminars, and in particular the hands-on workshops, are very useful in exposing the user to high performance computing. Some users who are experienced in using the same software application on workstations or high-end PCs found that the training exposed them to the speed capacity of supercomputers and encourage them to "think big" when they returned to their companies. This helps to overcome the resistance in accepting a new technology.

Company Visits

While seminars and workshops is one avenue for NSRC to reach out to Singapore organisations, participants are usually cautious about discussing engineering problems in a public setting. Therefore, NSRC organises small teams of 2 - 3 persons to visit the companies at their office where possible. In-depth details about problems and solutions are usually revealed during such meetings.

In the past two years, NSRC has made contacts with over 100 organisations in Singapore and organized company visits to about a dozen of them. Major R&D organisations in Singapore have been covered, including :

- Institute of Systems Science
- Information Technology Institute
- Defence Science Organisation
- Economic Development Board
- Singapore Productivity and Standards Board
- GINTIC Institute of Manufacturing Technology
- National Computer Board
- Dept. of Engineering, NUS
- Dept. of Information Systems and Computer Science, NUS
- School of Applied Science, Nanyang Technological University
- Port Authority of Singapore

One issue that frequently surfaced in such visits is security. Companies are wary of putting CAD designs or plant layout on machines which are openly accessible, particularly one that is open to the Internet. In view of this, NSRC implemented the following security measures:

- Multi-Level Security (MLS) on the Cray
- Security policy for all NSRC staff
- Regular security audits
- Internet Firewall with SecurID.

Work with Relevant Organisations

NSRC application staff plays the role of a bridge between the problem the users are trying to solve and the machines that are

available. They are therefore required to have some domain expertise on the user's problem, and at the same time be able to translate the problem so that it can be tackled on the computers. Users are expected to have the basic understanding of modelling and simulation; these users will have the most benefit when they work with NSRC staff. Users who are completely new to computer modelling and simulation are channelled to the relevant organisations for more in-depth assistance.

The reason is simple: with a staff of 30 supporting eight application areas, a host of users, and operating 3 supercomputers, it is impossible to cover all eight application areas to a great depth. Many such application-specific research organisations exist in Singapore. For example, structural analysis and plastic injection molding users can be encouraged to work with the Precision Engineering Development Centre (PEDEC), another government funded organisation focused in precision engineering application such as metal stamping and injection molding.

Leverage on Cray Application Analysts

As part of the acquisition of NSRC's Cray T94, NSRC is entitled to 6 man-months of Cray Application Analysts' time. This is an extremely useful source of expertise to achieve technology transfer to Singapore. Again, NSRC organises seminars and/or workshops jointly with Cray Application Analyst where they can teach Singapore users about the state-of-the-art in the application of high performance technology.

A list of visits in 1996 by Cray Application Analysts is given in the table at the end.

Current Status

Currently, NSRC has about 180 accounts on all three supercomputers. Utilization ranges from 61% on the NEC SX3 to 68% on the Cray T94. With this user base in mind, problem reporting has to be tracked more systematically. Enhancements to NSRC's Web site to take advantage of the full capability of the World-Wide Web is also being planned. Singapore is clearly in a catch-up position when NSRC is set up 3 years ago. Significant progress has been made, but there is still a long way to go.

	Application	
Date	Analyst	Activities
September 1996	Dr Longwu Wu	"5-day Workshop on Sheet Metal Forming Simulations on the Cray T94 Supercomputer" - 9 - 13 Sept
September 1996	Dr Carlos Sosa and Mr Chee- Keong Lee	"Introduction to Gaussian : Theory and Practice" - 2 - 5 Sept Visited users
August 1996	Dr Michael Y Sheh	"CAE for sheet metal forming" - 13 Aug Visited 3 companies
June 1996	Dr Luca Zullo	"High Performance Computing for the Process Industries" - 24 June Visited 3 refineries
May 1996	Dr Cal Kirchhof	"The Importance of Visualization in Supercomputing" - 28 May
May 1996	Mr Chee-Keong Lee	"Introduction to Ensight and Hexar" - 16 - 17 May
April 1996	Dr Longwu Wu	"The Use of Computer Aided Engineering (CAE) Tools in Sheet Metal Forming Industries" - 1 April Visited 3 companies
January 1996	Mr Michael Aamodt	"Supercomputing in the Electronics Industry" - 2 Feb