



Outreach

The HPSC is re-organising to improve the delivery of benefits into CSIRO science from the provision of high performance computing capabilities. These changes are intended to:

- Help CSIRO scientists adopt computational and data management capabilities
- Support scientists in achieving performance from scientific codes and application suites
- Engage grid infrastructure development in the broader Australian eResearch environment
- Support a closer integration of HPSC developments with CSIRO-IT

To drive home that change, two new positions have been established and the division of responsibility between running systems to support science activity and integrating the needs of existing and new users of computational science is now part of our structure.

Rob Bell continues as the HPCCC Chief Technical Officer, responsible for systems operations. Gareth Williams will become the “Manager, HPSC Outreach”. In that position, Gareth will:

- Identify power user needs (science goals where HPSC is a critical-path input), and assist HPSC and other resource providers to meet those needs
- Assist the integration of HPSC facilities with CSIRO-IT facilities and, in particular, ensure there is seamless access to HPSC facilities from the CSIRO desktop
- Lead HPSC’s involvement in APAC projects and other grid activities within the emerging Australian eResearch infrastructure

In addition, Alf Uhlherr, will be seconded from Molecular Science, into the “Manager, Science Strategy” role to assist HPSC evaluate and revamp its service offering. Alf will:

- Compare CSIRO’s use of HSPC with similar organisations to map science needs
- Identify additional power user groups and the capabilities that might meet their needs
- Promote services from HPSC to CSIRO Scientists and divisional managements

Power user story

As part of our revamp in service delivery, HPSC is providing new forms of support arrangements, and we would be very happy to partner with other research groups in similar ways.

In this particular case, CSIRO, through Marine and Atmospheric Research, is participating in the BLUElink ocean forecasting project <http://www.marine.csiro.au/bluelink/> with the Bureau of Meteorology and the Australian Navy. One part of that project involves the delivery of a forecasting model along with the computer systems able to support that forecasting.

Following negotiations with the divisions, a cluster dedicated to the ROAM model is now hosted within the HPSC facilities, providing ultra fast access to other systems and the large HPSC Datastore. We were able to assist with the requirements specification, procurement process, installation, acceptance testing (leading to additional hardware supplied by the vendor to meet benchmark requirements) to produce a dedicated facility supporting the project.

Importantly, the compute resource is a divisional asset with exclusive access by the project. HPSC provides cost efficient management and user support as a contribution to the project. In addition, the research team have the benefit of access to a similar additional cluster and other systems that are HPSC assets available to all CSIRO staff on a shared basis.

MSC Software update

HPSC now provides access to the full complement of MSC software, upgraded to the 2005 versions, as well as CFD-Ace, Ensignt and Gaussian. Apart from Gaussian, the licence arrangements allow for most components to execute on any CSIRO system and the token based system provides for optimal sharing of licences across the organisation. HPSC recovers a nominal \$5,000 per annum for a single user and \$10,000 per annum for a research group access, to cover growth in license fees which rise with volume of use.

Groups already signed include CMIT using Marc, Mentat, Patran and CFD-ACE, and Exploration & Mining and Forestry & Forest Products using Patran. Our experience is that establishing the optimal environment for each use can take a few weeks of trial and testing. Researchers interested in any MSC software should contact Len Makin.

Systems Upgrades

Several of the systems in HPSC have been upgraded over the last two months:

- Additional processors have been delivered for the Xeon clusters
- Additional memory in the HPSC Xeon cluster, up from 2Gbyte to 4Gbyte per node
- Speed increase on the Altix, Itanium2 processors upgraded from 900MHz to 1.3GHz
- Additional memory in the Altix means we can now run jobs in up to 180Gbytes of RAM

Further upgrades in compute power and storage density are planned for early in 2005.

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