



SX-5s shutdown

Finally the old vector supercomputers, the SX-5s, have been retired. The machines were purchased in 2000 and have now been replaced by a much larger configuration of SX-6 vector nodes located at the new HPSC site. Rob Bell on the right and some of the other CSIRO, BoM and NEC staff who attended the “big switch off” are pictured below waiting patiently for the machines to wind down (the big red button which does exist is unfortunately obscured by Rob).



Scientific Software

Recent feedback has underscored the fact that high performance software as well as hardware capabilities are needed to assist CSIRO staff make best use of computational resources.

Consequently we propose to establish a repertoire of software applications on HPSC facilities and to provide some that will be more widely available across CSIRO. Initial steps are outlined below, and we are very interested to identify additional key needs.

It is important to appreciate that HPSC's role means that the software solutions are configured to support high end computational needs and, while they will integrate where possible with desktop science needs, their provision and configuration is not aimed at the desktop.

Cost sharing

One of the difficulties in providing software access is that licence fees grow with use so that some contribution is needed to meet cost growth. While it would be possible to attach differential cost sharing arrangements for each component, the HPSC proposes to make access to all its licenses on a simple fee per user, where the fee makes a contribution towards the provision of the licences.

The proposed user contribution is \$5000 per year for a staff member to make use of any and all HPSC software. Some groups have asked if a single seat could be shared amongst group members. We believe that such an arrangement may be possible within the license server, and if so, would like to negotiate an appropriate contribution on a case by case basis.

Contributions will be expended on licences and user support and an accounting of costs incurred and fees received will be provided at the end of each year to all participants.

Gaussian

The HPSC will provide a queue delivering a Gaussian computational engine running on a full SX-6 node (delivering 64 Gflops vector SMP). An additional Gaussian computational engine will be supported on the Altix.

Unfortunately the licence for desktop GaussView is site based, which appears to be most related to the concept of a physical building. HPSC will provide a site licence that can be executed at its premises and will provide additional site licences where required.

MSC Software

The HPSC proposes to provide shared access to all MSC software through a central licence server. This is a complex offering for a range of software related to solid modelling and manufacturing design.

The complexity arises because the arrangement:

- will allow MSC software to be executed on divisional as well as HPSC systems
- is a volume purchase so that costs increase with usage
- requires HPSC to configure batch access to computational engines as need arises

Consequently, this represents many unknowns in software management and system configuration and the HPSC would request some tolerance as the entire package comes on line.

CFD-ACE+

The HPSC will provide a queue delivering a CFD-ACE computational engine running initially on a four processor subset of the Altix (delivering 20 GFlops SMP) as well as access to three licenses for CFD-GEOM and CFD-VIEW able to be accessed through the MSC licence server.

Other Software

HPSC is looking for scientific staff to assist identify the range of software needed to exploit large computational and data resources, please contact Len Makin in the first instance. Access to EnSight will be available under the MSC license server and the Altix will have Mathematica.

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