

SCIENTIFIC AND TECHNICAL ADVISORY COMMITTEE

Minutes of the 5th Meeting

Monday 20th January 2006

By Access Grid from UCL

PRESENT:

Richard Catlow (CRAC) - Chair
Rudiger Esser (RE) - via AG from Juelich
Martyn Guest (MFG)
Damian Jones (DJ) - Secretary
Charles Laughton (CL)
Linda Sayers (LS)
Alan Simpson (ADS)
Lois Steenman-Clark (LSC)

APOLOGIES:

Sam Falle (SF)
Mike Leschziner (ML)
Ralph Roskies (RR)
Mark Sansom (MS)

1. Welcome (CRAC)

The Chairman, CRAC, welcomed the members of STAC - and informed everyone of a new member of the committee, Prof Sam Falle from Leeds, who will be taking the place of Carlos Frenk who has resigned his position. Unfortunately Prof Falle is unable to join the meeting today because of AG problems.

The minutes of the previous meeting, held on the 28th September 2005, were accepted as a true record.

2. Minutes and Actions of the Previous Meeting

- Joint website between HPCx and CSAR to display the publications / scientific highlights information - This will be discussed later in the agenda.

ACTION COMPLETE

- LS to feedback our concerns over the delay in approving the Annual Plan to Hugh Pilcher-Clayton. - CRAC had spoken with Hugh about this matter, as had LS. Hugh felt that the problem was a delay in HPCx getting the report to him in the first place, not the other way around. ADS thought that this was not the problem. Hugh was sent the Annual Plan by 1st March 2005 but it was not approved until August 2005. Hugh will have this year's Annual Plan in the next couple of weeks, following any amendments made to include the recommendations from this STAC meeting. We would like to aim for approval by the end of April or even by the end of March following the next Oversight Committee meeting on 15th March. LS to feedback to Hugh Pilcher-Clayton.

ACTION ONGOING: LS to speak to Hugh about the timelines suggested by STAC for approving the 2006 Annual Plan

- ADS to canvas Users to discover which topics would be most useful if they were covered by a Technical Report. - This will be discussed later in the agenda.

ACTION COMPLETE

- STAC to comment on the targets set in the 2006 Annual Plan. - This will be discussed later in the agenda.

ACTION COMPLETE

- CRAC to contact Ian Green, on behalf of STAC, for feedback on the IBM "HPCx Planning Workshop". - The head of the PESSL development team had responded saying that what we were asking for wouldn't be available until the next release (Q1 2006). That release arrived about 3 weeks ago and it seems a lot better. There is a definite improvement. It is noted that there has now been some progress on this matter.

ACTION COMPLETE

- DJ to include an agenda item to discuss the final visit report at the next STAC meeting. - This will be discussed later in the agenda.

ACTION COMPLETE

- DJ to look for dates for the next STAC meeting in February 2006.

ACTION COMPLETE

3. Annual Report 2005 (ADS)

ADS gave a progress report on the HPCx service during 2005.

- Upgrade to POWER5 – Phase2 was replaced with a POWER5 based system in Q4 2005 (Phase2A). This was a very successful change over with minimal disruption to users, thanks to a lot of hard work by IBM and the HPCx Systems Team. Benefits of Phase2A include enhanced memory (2x memory per processor and almost 2x memory) and enhanced performance for user codes (on average 50% faster than Phase2 benchmark tests). We also now have an additional development system through a contribution from NERC

(128 POWER5 processors / 10TB's of disk), which is linked to Phase2A but has a separate queuing structure.

LS-C stated that the change over from Phase2 to Phase2A was incredibly smooth and CRAC asked that thanks be passed on to all the Systems Team involved.

- Capability Science – HPCx was involved in the SPICE project, which won the HPC Analytics Challenge Award at SC05 in Seattle. We have also completed some Soft Matter work, which was published in 'Science'.
- Other highlights for the year included a very successful training programme (new and updated courses), an independent security audit completed by QinetiQ, and various conferences (ScicomP, SP-XXL, SC05, ISC05 etc).

ADS highlighted the utilisation figures, split by research area. Total utilisation averaged around 75% for the year. There has been growth in usage from the Environment and Life Sciences areas, which CRAC identified as a "pleasing development". There are some issues around support for new users, especially those coming from CSAR when their service closes in June 2006, and the number of consortium that are using the system. We currently have over 40 consortia using the service. There is some concern that this will have a knock-on effect on the work we can do and the quality of service we can provide.

Capability Usage has also seen significant growth during 2005, up to 57% in December which is the first month we have gone above our target of 50%. However, the two biggest capability users on the system have now finished their grants so the number will fall again during the early months of 2006. There are still a limited number of consortia dominating capability usage. LS-C stated that the incentives for capability usage are not attractive enough at present to encourage groups to put the effort in to reach capability usage. These rewards need to be looked at if we are going to encourage more groups to pursue capability usage. It was agreed that we should send some feedback to Hugh that there needs to be a more dynamic review process to encourage capability usage in the future.

ACTION: CRAC / MFG to devise some recommendations on how we could encourage capability usage that can be circulated to STAC for comment.

LS mentioned that an allocation panel might be a good idea for HPCx. MFG highlighted the disconnect between the HPCx Oversight Committee and STAC, and the fact that there is no scientific representation on the Oversight Committee, except Patrick Briddon. HPCx should examine the advantages/disadvantages of an allocation panel or a Directors discretion scheme.

The Performance Metrics for the year were shown and they highlighted the fact that HPCx exceeded Full Service Levels for every metric during 2005.

ADS then highlighted the progress and successes against the Key Objectives for the year.

1. Capability incentives for at least 5 codes - during 2005 six codes reached gold status and one code reached bronze status.
2. Scientific delivery and research outcomes – we now have a joint web site with Manchester which can be accessed through the HPC-UK web pages.
3. Investigate key areas for Capability computing – we developed a production-quality library optimising alltoallv (S.Booth), updated Globus for HPCx and produced a Technical Report on I/O performance on HPCx.
4. Demonstrators of capability computing – HPCx was involved in the SPICE project at SC05.
5. Outreach – HPCx is supporting the current lifesciences projects (such as CCPB), marketing HPCx to the industrial community (AstraZeneca and OHM Surveys), improving public awareness (Edinburgh Science Festival, Daresbury Laboratory 25 year Anniversary Celebrations), supporting Grid projects (co-investigators on SPICE), and visualisation.
6. Evaluate code and performance portability – current research underway into portability from HPCx to the Edinburgh BlueGene system.
7. Produce at least twelve Technical Reports – twelve reports were produced, with two accepted for journal publication.
8. Adapt training programme to benefit users – we delivered our target of thirty course-days. Sixteen courses were held on four different sites around the UK We also held multiple runs of core courses and developed and ran three new training courses.
9. Ready access to information – the HPCx helpdesk met all targets, documentation is updated regularly on web, and two User group meetings were held during the year.
10. Ensure support effort is dominated by experience staff – 100% of full service level was delivered from named experienced staff.

CRAC commented that the report represents a very satisfactory and successful year for HPCx and shows that we have responded to comments and issues raised by STAC.

4. Annual Plan 2006 (ADS)

ADS gave an overview of the Annual Plan for 2006. He outlined the challenges - such as the drop in Science support staff from 13 to 10 and the addition of users and data from CSAR - and the opportunities - Phase 3 and DEISA / Europe - for HPCx in 2006

The initial draft of the key objectives for the year has been approved by EPSRC and the Oversight Committee...

1. POWER5 - we will undertake activities to ensure that new users can effectively exploit the new POWER5 processors.
2. Capability Incentives - we will collaborate to obtain improved capability incentives for at least four established codes and further analyse the potential for enhanced incentives from the top codes on Phase2A.
3. CSAR - we will aim to minimise the problems that users face when they migrate to HPCx from CSAR through training courses and workshops.

4. Europe - we will take a more significant role in DEISA. Five percent of the system has been allocated for the DEISA project. RE confirmed that Juelich offers time on their system to fellow European partners but it was noted that at the present time HPCx would have problems with being able to offer similar.
5. Capability Exemplars – we will capture two demonstrators of science-driven exemplars.
6. Portability – we will evaluate potential code and portability problems for HPCx codes moving to other systems.
7. Ease of Access – we will reach out to the user community to allow ease of access to HPC support expertise.
8. Software Trends – we will evaluate trends in software areas that may require enhanced support in the future.
9. Outreach – Life Sciences funding is ending so there will be limited resources available. We will, amongst other things, publish scientific outputs via newsletters, conferences and seminars, and will support Grid projects that are exploiting HPCx.

CRAC mentioned that Special Editions of current journals are a good way to publish scientific outputs that are well received by the community.

10. Technical Support – we will have the following targets for 2006: ten technical reports and twenty five days training.
11. Science Support Staffing – we will deliver 80% of the FSL effort levels from named experienced staff.

ADS concluded by summarising the four areas that HPCx will focus on in 2006...

- Producing capability science from POWER5
- Ensuring high quality research outputs
- Exploiting European Grid opportunities
- Supporting users transferring from CSAR

LS-C asked that next year's objectives highlight the fact that HPCx is the only facility of its kind in the UK following the closure of CSAR.

CRAC concluded this section of the meeting by confirming that STAC supports the 2006 Annual Plan and by asking ADS to go ahead along these lines, especially around the four objectives outlined in his summary above.

5. Consortium Visits (MFG)

MFG gave a brief overview of the Consortium Visits report that had been circulated before the meeting. The site visits will continue during 2006 because it has been recognised that a lot can be learned by meeting with, and talking to, the Groups. One issue raised during the site visits completed in 2005 was the limits of memory on the system which have been addressed with the recent Phase2A upgrade.

CRAC agreed that the site visits programme was a very useful exercise that was appreciated by the consortium members and should continue in the future. The whole exercise was extremely valuable.

6. Benchmarking Phase2A (MFG)

MFG gave an overview of the performance of Phase2A. He highlighted a chart in his presentation showing performance ratios for the acceptance test codes from Phase2 to Phase2A. Most codes showed an improvement, except the molecular dynamics codes such as DL_POLY, AMBER, NAMD etc. This may be a memory latency problem and is being examined in more detail.

7. Benefits of Additional Memory (MFG)

MFG spoke very briefly to a paper written by the HPCx Terascaling Group on the impact of the HPCx Phase2A memory upgrade.

8. Any Other Business

There was no other business.

9. Date of Next Meeting

It was suggested that the next meeting should take place in early September 2006 and that it would be held at UCL (by Access Grid). DJ will look for availability.

ACTION: DJ to look for dates in early September 2006.

*Damian Jones
22nd February 2006*