

## SCIENTIFIC AND TECHNICAL ADVISORY COMMITTEE

### Minutes of the 3<sup>rd</sup> Meeting

Tuesday 1<sup>st</sup> March 2005

By Access Grid

#### **PRESENT:**

Richard Catlow (CRAC) - Chair  
Patrick Briddon (PB)  
Martyn Guest (MFG)  
Damian Jones (DJ) - Secretary  
Charles Laughton (CL)  
Alan Simpson (ADS)  
Lois Steenman-Clark (LSC)

#### **APOLOGIES:**

Ralph Roskies (RR)  
Michelle Vail (MV)

### 1. Welcome (CRAC)

The Chairman, CRAC, welcomed the members of STAC.

The minutes of the previous meeting, held on the 30<sup>th</sup> September 2004, were accepted as a true record.

### 2. Minutes and Actions of the Previous Meeting

- MRC Representative - Charles Laughton from the University of Nottingham had accepted the position and was in attendance at this meeting. **ACTION COMPLETE**
- PI's to provide an updated list of publications for their consortium every six months plus one or two scientific highlights - This action will be discussed later in the agenda. **ACTION COMPLETE**
- Joint website between HPCx and CSAR to display the publications / scientific highlights information - This action is in progress and will be discussed later in the agenda during MFG's presentation. **ACTION IN PROGRESS**

- Discuss possibility of joint website with CSAR - This action is in progress and will be discussed later in the agenda during MFG's presentation. **ACTION IN PROGRESS**

### **3. Annual Report 2004 / Annual Plan 2005 (ADS)**

ADS delivered a presentation on the HPCx Annual Report for 2004 and the Annual Plan for 2005.

Annual Report 2004 - CRAC commented that the report highlighted another successful year for the service. The major issue for the year had been capability computing.

A question was raised by PB about the IBM Workshop held in May 2004, and in particular the actions that IBM had agreed to reply to during that Workshop. It appears that IBM have still not completed their actions from that Workshop. MFG / ADS will mention this at the next HPCx Oversight Committee meeting and will explain to the committee that STAC would like to see delivery of the agreed package of software improvements. They will also speak with the relevant people at IBM and will report back at the next STAC meeting.

**ACTION: MFG / ADS to speak to IBM about the progress of their actions from the IBM Workshop held in March 2004. MFG / ADS to raise STAC's concerns at the next Oversight Committee.**

LSC spoke about her concerns that the service may never reach its capability targets. MFG explained that he would speak about this matter during his presentation later in the agenda, however, there is also a long standing action with EPSRC to discuss the metrics and definition of capability computing in relation to the HPCx service. ADS / MFG to speak with EPSRC.

**ACTION: ADS / MFG to discuss the metrics used to define capability computing with EPSRC.**

Annual Plan 2005 - LSC raised the issue of defining the metrics used to quantify scientific quality, in particular in relation to objective two from the list of science support objectives. MFG suggested that the process of defining the metrics cannot lie solely with HPCx. The process must also involve EPSRC, with possible input from the TOP and TWP sub-committees of HSC. CRAC agreed with this statement.

CRAC enquired about the five codes that would be selected to fulfil objective one (*Obtain capability incentives for at least five codes from a range of areas*). CL expressed concern with focussing on just five codes, suggesting that HPCx could broaden its user base by increasing the number of codes that it focussed on. MFG agreed that there is a need to enhance a broader code base, but suggested that the number of codes that HPCx could realistically focus on is limited given that the primary metric used by EPSRC is capability usage. ADS pointed out that if we decided to focus on ten codes instead of five then, because of pressures on staff, other areas may be neglected. It is important that we get the balance correct. CRAC summarised the discussion by pointing to the importance of the planned consortia

visits in identifying the five codes to be selected. He pointed to the real tension between promoting capability computing and broadening the HPC user community, and suggested that this concern by STAC should be fed back to the Research Councils.

CRAC also enquired about industrial contacts. ADS explained that EPSRC have a project success metric where HPCx has to show some industrial usage. HPCx is currently looking at some opportunities but it is not one of the major concerns. RE agreed with this approach and confirmed that in Germany they see the same trend as we are seeing now - industry is not that interested and the effort you put into making contacts is not worthwhile. MFG added that a number of software companies associated with commercial codes on the system (CFX, FLUENT) have indicated that some of their customers may be interested in making use of HPCx in the future.

CRAC felt that the forthcoming talk at the Edinburgh Science Festival is a positive effort towards outreach activities. ADS will report back at the next STAC meeting.

**ACTION: ADS to report back on outcome of Edinburgh Science Festival.**

RE enquired about the type of systems that we would be looking at in the future (objective five). ADS explained that the future of HPC looks very interesting, with new architectures at NEC and CRAY, as well as the next generation IBM and SGI systems.

CL felt that objective eight (Outreach activity) was very important and should be moved up the list of objectives. Although it had moved up from number ten last year to number eight this year, STAC felt it should be moved up higher.

**ACTION: ADS to move objective eight up the list of objectives.**

CRAC concluded that the general feeling was that STAC agreed with the objectives outlined in the Annual Plan for 2005. The main priority for the year has to be attaining capability computing but with some consideration for broadening the User base. It is also important to raise the importance of outreach activities. These conclusions should be passed onto Hugh Pilcher-Clayton at EPSRC.

**ACTION: CRAC to pass on the conclusion of STAC's discussions to Hugh Pilcher-Clayton.**

#### **4. Capability Science (MFG)**

MFG gave a presentation on Enabling Capability Science on HPCx.

CRAC was pleased to hear that capability usage has risen again in February but questioned how we can stabilise these figures.

LSC highlighted the fact that CASTEP accounts for 30% of the usage figures but does not scale. If this could be addressed then many of the current problems with capability usage could be solved. LSC also pointed out that the practice of using the number of processors as the metric for defining capability usage is the problem. Lots of good science has been produced from CASTEP using 128 processors but this is not classed as "capability computing" given the current metrics. MFG agreed with LSC's

observations and explained that the users have chosen to use CASTEP over various other codes that scale better but offer similar functionality.

ADS explained the reasons behind the suggested trial of the new queue structure, which will hopefully help to stabilise the capability usage. This trial will be over a six month period if approved by EPSRC. LSC expressed some concerns over the trial that MFG agreed could be addressed if major problems arise. PB agreed that the trial would be a good idea but may lead to problems with areas of the capability partition system likely to be unavailable to users given the large processor counts involved. It is easier to allocate small jobs than large ones.

CRAC summarised the discussion by stating that STAC supports the proposed trials but that the committee understands LSC's concerns. If the trial is approved at the next Oversight Committee ADS will report back on progress at the next STAC meeting.

**ACTION: ADS to report on progress of the revised queue structure.**

CRAC asked if consortia had been selected for site visits. MFG explained that the process was currently underway and agreed to report back at the next meeting.

**ACTION: MFG to report on progress of site visits.**

CRAC concluded this section of the agenda by stating that STAC supports the proposed measures designed to increase capability usage on HPCx.

## **5. Any Other Business**

CRAC summarised the view of STAC that there a number of important issues that needed consideration with EPSRC, particularly in light of the forthcoming HECToR service. The committee agreed that the chairman should contact Hugh Pilcher-Clayton outlining these issues and the associated concerns of STAC. This interaction would then hopefully lead to a face-to face meeting between CRAC / ADS / MFG and Hugh Pilcher-Clayton where the issues could be discussed in more detail.

**ACTION: CRAC to contact Hugh Pilcher-Clayton on behalf of STAC.**

## **6. Date of Next Meeting**

It was suggested that the next meeting should take place early in September 2005 and that it would be held at UCL (by Access Grid). DJ will look for availability.

**ACTION: DJ to look for dates in September 2005.**

*Damian Jones*  
*2nd March 2005*