

SCIENTIFIC AND TECHNICAL ADVISORY COMMITTEE

Minutes of the 2nd Meeting

Thursday 30th September 2004
Room 205, University College London

PRESENT:

Richard Catlow (CRAC) - Chair
Martyn Guest (MFG)
Jennifer Houghton (JH)
Damian Jones (DJ) - Secretary
Mike Leschziner (MS)
Alan Simpson (ADS)
Lois Steenman-Clark (LSC)

APOLOGIES:

Patrick Briddon (PB)
Ralph Roskies (RR)

1. Welcome (CRAC)

The Chairman, CRAC, welcomed the members of STAC who were in attendance at UCL, and apologised for the problems with the Access Grid that had prevented the members of the Committee who were not in attendance from joining the meeting.

2. Minutes and Actions of the Previous Meeting

- MRC Representative - The MRC representative on STAC, Hooshang Nikjoo, had resigned and a replacement needed to be identified. Contact had been made with Charles Laughton at the University of Nottingham, who had been the co-applicant on Nikjoo's Life Sciences proposal. Laughton had agreed in principle to join STAC but would like more details and the Terms of Reference before committing himself. It was hoped that Laughton would join STAC at the next meeting. **ACTION IN PROGRESS**
- HPCx Metrics - RR had questioned the metrics defined in the review of the first year of the HPCx service and had asked whether these would be refined

for the second year. There had been some interaction between ADS and RR over this matter but the basic metrics would remain the same. **ACTION COMPLETE**

- Workshop to Improve Dialogue Between NERC and HPCx - A workshop had taken place involving the NERC consortium. This item will be discussed in more detail during ADS's presentation later in the agenda. **ACTION COMPLETE**
- Promoting and Disseminating Work on HPCx - This matter has been addressed and will be discussed during ADS's presentation later in the agenda. **ACTION COMPLETE**
- Progress Report on the Life Sciences Programme - This matter will be addressed during MFG's presentation later in the agenda. **ACTION COMPLETE**

3. The Phase 2 Upgrade (ADS)

ADS delivered the presentation on the Phase 2 upgrade that had been circulated to the committee. The presentation comprised a general overview of the recent upgrade to the system.

LSC commented that the transition was very smooth from a User perspective. CRAC asked that congratulations be passed to the team involved in carrying out the successful transition.

4. Usage / Capability Usage (ADS)

ADS delivered the presentation on usage of the system that had been circulated to the committee. ADS explained to the committee that HPCx had recently agreed with EPSRC to raise the number of consortia from 30 to 40.

CRAC pointed out that it was encouraging to see that the science base on the system is growing.

5. Progress Against the Annual Plan (ADS)

ADS delivered the presentation on progress against the annual plan that had been circulated to the committee.

LSC commented on the workshop that had taken place to improve dialogue with the NERC groups. This had been a very useful meeting. One problem that had been identified was the need for extra disc space for the NERC codes. Jobs were crashing on the system because they were reaching their disc quota limit. ADS explained that this problem could be addressed. Extra disc space is available on the system - the

NERC consortia should put a request for higher quotas into HPCx for consideration. LSC will report this back to the NERC groups.

CRAC commented on the three presentations that ADS had given to the committee. He noted that it had been a successful year for the service and that it was good to see that HPCx had responded to the suggestions of STAC. The focus should remain on capability computing, with consideration of the metrics used to define capability computing.

6. Performance of Phase 2 (MFG)

MFG delivered the presentation on the performance of phase 2 that had been circulated to the committee.

LSC enquired about an implementation date for SP9 and MFG explained that following the recent last-minute problems with the scheduled release of SP9 no new date had been provided by IBM, although he expected it to be quite soon.

LSC also asked if there was any indication of IBM's future plans following SP9. There has been no explanation of IBM's future plans but it was felt that it was important to have some input from the terascaling team at HPCx - not just from IBM.

CRAC commented that the performance figures on Phase 2 looked encouraging.

7. Scientific Highlights (MFG)

MFG delivered the presentation on scientific delivery that had been circulated to the committee.

JH commented on the fact that it was very difficult to get feedback from the User community when it is asked for, eg - the lack of response to the recent request for a list of publications. ADS explained that part of the problem may be the lack of incentive for the PI's to provide the information.

CRAC suggested that every 6 months the PI's should provide an updated list of publications for their consortium plus one or two scientific highlights. These could then be displayed on the Web, with STAC providing a "Top 10". It was felt that the request for his information should come from EPSRC rather than HPCx.

ACTION: JH to discuss this suggestion with Hugh Pilcher-Clayton and report back to STAC.

It was felt by the committee that if this approach was adopted then there should be a joint website between HPCx and CSAR to display the information, or the information should at least be cross-linked between websites. It was not appropriate to display on the EPSRC website or to display it just on the HPCx website.

ACTION: ADS to look into the possibility of creating a new web page to display the information - using a domain name such as "www.hpc.ac.uk".

It is also important that this suggestion is discussed with CSAR.

ACTION: JH / ADS to discuss the idea of a shared website with CSAR.

MFG concluded by providing the committee with an overview of the current status of the Life Sciences programme:

- Mark Sansom's project is now up and running. He is currently benchmarking five different molecular dynamics codes,
- Marcus Durant from the John Innes Centre has a project that is in the advanced planning stage.
- Adrian Mulholland's project, "*Modelling enzyme catalysis: activity, stability and dynamics*" has now started.

8. Any Other Business

None.

9. Date of Next Meeting

It was suggested that the next meeting should take place in Mid-February 2005 to follow the submission of the Annual Plan, which is due in January 2005. It was also suggested that the meeting should take place in Edinburgh where a dedicated Access Grid operator would be available to ensure that there was not a repeat of the problems encountered today so that the overseas members of the Committee could join the meeting. DJ will look for availability for February 2005.

Damian Jones
1st October 2004