

Summary of Annual Plan for Science Support and Capability Computing 2005

1 Overview of Themes

Having successfully implemented the transition to Phase 2 during 2004 with minimal disruption to users, the focus of the HPCx service for 2005 will be on delivering capability science. The HPCx system and support activity are now both in a mature state and the success of the project will inevitably be judged on the quality of the research outputs over the next two or three years.

The Phase 2 hardware has shown itself to be quite reliable during the last six months and a wide range of codes have been able to demonstrate good performance and scaling. However, the trend in capability usage has not been so encouraging. We intend to work closely with key consortia to address any barriers to capability computing and encourage them to focus on world-class calculations.

The focus on capability science will require a number of different activities involving all the Science Support teams and the Systems team. These will include:

- Ensuring key applications effectively exploit hundreds of processors;
- Working with users to demonstrate the scientific outputs;
- Facilitating world-leading capability demonstrators;
- Promoting public understanding of capability science;
- Investigating general terascaling and performance optimisation techniques;
- Ensuring capability computing courses and reports are readily available;
- Data handling and the Grid;
- Tuning the system configuration to maximise throughput of capability jobs;

These activities should maximise both the capability computing and the delivery of high-quality science outputs. HPCx is a major opportunity for the computational science community and we will aim to ensure that the UK realises the research benefits of this facility.

2 Key Objectives

The following points represent our specific key objectives for 2005, in approximate order of priority.

1. During the course of this year, we will endeavour to obtain capability incentives for at least five codes from the following range of areas: Chemistry, Material Science, Environmental Science, Engineering and Physics.
2. Working with the consortia, we will look to generate an updated account of scientific delivery and research outcomes from HPCx. Our goal is to generate an on-going record of scientific highlights, driven by a series of associated metrics e.g., publications, presentations, citations etc. We have been encouraged by STAC to pursue what is recognized to be a key activity in promoting the scientific impact benefit of HPC.
3. To underpin the applications-focused activities, we will also investigate a number of key areas for capability computing:
 - General terascaling and optimisation techniques;
 - Advanced data handling and the Grid.
4. Facilitate at least two high-profile world-leading calculations as demonstrators of capability computing. Likely candidates include the successful bidders for the joint US-UK High End Computing Projects bid for experiments at SC2005.
5. Evaluate potential code and performance portability problems for HPCx codes moving to future systems.
6. Produce at least twelve technical reports covering capability computing and related topics as discussed in 2.1.2, with the following number of reports in each quarter: 4 (Q1), 3 (Q2), 3 (Q3), 2 (Q4).
7. We will continue to adapt the training programme to benefit users and promote all aspects of capability computing. Key elements include:
 - Focusing on the core courses relevant to capability computing;
 - Running a tailored version of the existing Scientific Visualisation course covering the use of VTK on HPCx;
 - Developing two new courses, one covering parallel IO and the other in an applications-specific domain;
 - Offering easy access to training material by running courses in at least four different of locations.
8. The outreach activity will focus on the following key areas:

- Supporting the current lifesciences project as they move into production, expanding into new projects in the bioengineering area and seeking to develop community wide projects;
 - Marketing HPCx services to the industrial community;
 - Improving public awareness, in particular through engagement with science festivals;
 - Supporting Grid projects exploiting HPCx and seeking to undertake joint experiments with the Teragrid sites.
 - Developing visualisation activities with Consortia.
9. It is essential to ensure users have ready access to information on all aspects of the service. To this end we will:
- Continue to provide a prompt and accurate response to queries;
 - Keep the documentation portfolio up-to-date as possible;
 - Publicise the HPCx service to encourage uptake through coordination and participation in newsletters, user groups and events, including two applications-specific workshops and the annual seminar.
10. Ensure that the science support effort is dominated by experienced staff and that this experience benefits the other staff and the user community at large.

