

# HPCx Quarterly Report

## July – September 2005

### 1 Introduction

This report covers the period from 1 July 2005 at 0800 to 1 October 2005 at 0800.

The next section summarises the main points of the service for this quarter. Section 3 gives details of the usage of the service, including failures, serviceability, CPU usage, helpdesk statistics and service quality tokens. A summary table of the key performance metrics is given in the final section. The Appendices define the incident severity levels and list the current HPCx projects.

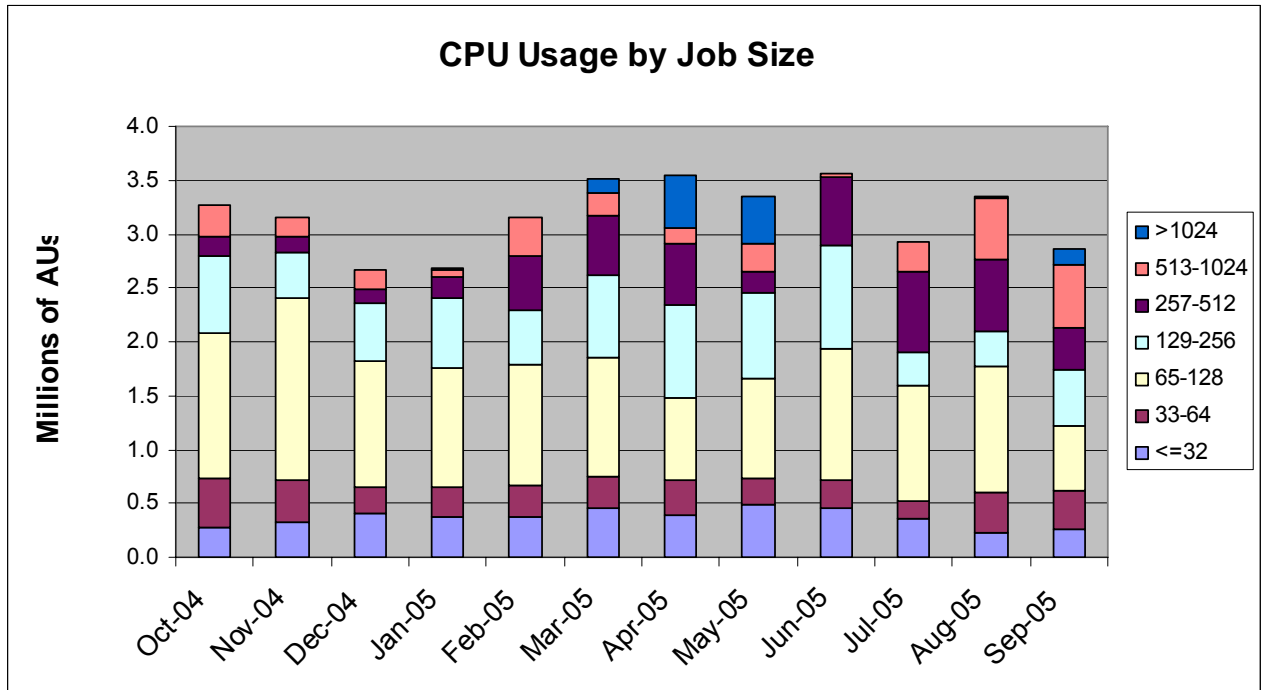
### 2 Executive Summary

- EPSRC have recently approved the upgrade of HPCx to a Power 5 system. The new system will be built up alongside the existing system during October and should go into service towards the end of November.
- The Annual Plan for 2005 was approved at the Oversight Committee meeting in August.
- Although overall utilisation has been more modest than the previous quarter, both capability usage (at 37%) and NERC usage (at more than 25%) have been high.
- The capacity-planning look-forward suggests that the HPCx system may be very busy over the next few months, as the e05 consortium have a lot of time to use before their end date of April 2006.
- With 5 new EPSRC consortia due to start in October, we are approaching the current maximum of 40 research consortia.
- After the successful talk at this year's Edinburgh International Science Festival, we have been accepted for next year's Festival. David Henty will give a talk titled *Supercomputers: rise of the machines*. We are also investigating participation in next year's National Science Week.

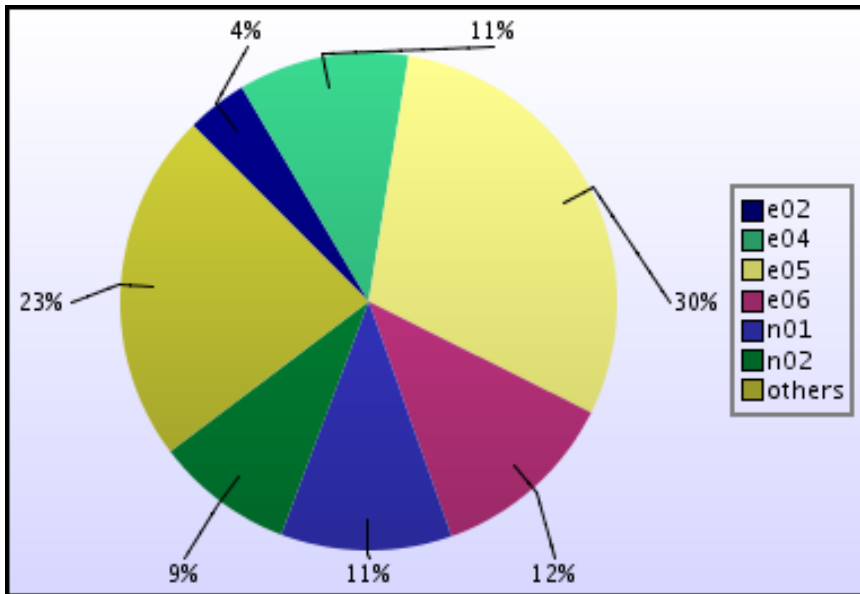
- Preparations are well under way for the SPICE and DYNOME experiments at SC2005 in Seattle. This has required work both on Grid-enabling codes and in updating of system software (port-forwarding and MPICH-G2).
- One of this quarter's HPCx Technical Reports, *On the Performance of Molecular Dynamics Applications on Current High-End Systems*, was published in the August 2005 issue of *Philosophical Transactions of the Royal Society of London Series A; Theme Issue on Scientific Grid Computing*.
- The summer provided an opportunity to run a good number of HPCx courses, bringing the training activity back on schedule for the year. The programme for the final quarter sees the development and delivery of four days of completely new training material for HPCx users.
- Organisation of The Third Annual HPCx Seminar, *Capability Science on HPCx*, is progressing well. The event will run at Daresbury on 5<sup>th</sup> December, immediately preceding the 16<sup>th</sup> Machine Evaluation Workshop.
- Martyn Guest wrote a paper based on the ten consortium visits carried out so far this year and made a presentation of the findings to the STAC meeting in September. This was well received by STAC and has demonstrated the value of these visits.
- This quarter has seen significant optimisation work on a variety of codes in different areas including: SCAM, GAMESS-UK, VASP and PDVR3DRZ. We have also ported to HPCx a number of other codes in support of the Life Sciences outreach activity.
- Significant testing of the new xlf9 compiler was performed on a wide range of codes prior to its roll-out to users in September. No problems were found and a number of codes obtained performance improvements. A presentation on the new features in the compiler was made at the HPCx User Group via Access Grid.
- As part of our investigation into future portability of performance, we have ported and profiled a variety of HPCx codes to BlueGene. These include the HPCx implementation test codes and other key HPCx applications. A presentation on this has been made available on the HPCx web site.

### 3 Utilisation

#### 3.1 By Job Size



#### 3.2 By Consortium



## 4 Summary of Performance Metrics

<i>Metric</i>	<i>TSL</i>	<i>FSL</i>	<i>July</i>	<i>August</i>	<i>September</i>
Technology serviceability	80%	99.2%	99.7%	100.0%	100.0%
Technology MTBF (hours)	200	300	732	∞	∞
Number of AV FTEs	7.5	10	14.4	14.9	14.1
Number of training days per month	22.5/12	30/12	13/7	20/8	20/9
Non in-depth queries resolved within 3 days	85%	97%	99.3%	100.0%	100.0%
Number of A&M FTEs	3.75	5.75	5.2	5.4	6.0
A&M serviceability	80%	99.6%	99.7%	100.0%	100.0%

<i>Colour</i>	<i>Meaning</i>
	Exceeds FSL
	Between TSL and FSL
	Below TSL

*Note 1:* The number of training days is reported as a running total since the start of the year.

*Note 2:* The above table includes the revised FSL targets for *training days* and *A&M serviceability*, which have been agreed with EPSRC.