

HECToR Quarterly Report

July - Sep 2010

1 Introduction

This report covers the period from 1 July 2010 at 0800 to 1 Sep 2010 at 0800.

Section 3 summarises service availability and performance statistics for this quarter. Utilisation statistics are also available in Section 3. A summary table of the key performance metrics is included. Section 4 shows Helpdesk statistics.

The Appendices define some of the terminology and incident severity levels and list the current HECToR projects together with their overall utilisation profile to date.

This report and the additional SAFE report are available to view online at <u>http://www.hector.ac.uk/about-us/reports/quarterly/3Q10.php</u>

2 Executive Summary

- XT utilisation in 3Q10 was 83.6%, compared to 75.3% in 2Q10. Further details are available in Section 3.2 of the report.
- Utilisation on the XT6 remains lower than we would like at 32.2% for the quarter. Although this percentage is low, more AUs were used on the XT6 than on the XT4 in 3Q10. The service now has far greater capacity and the challenge is to increase demand to meet this capacity.
- Charging rates on the XT6 have been reduced in order to provide some level of compensation for those users whose codes do not perform well on the current Seastar interconnect. These rates will be reviewed when the Gemini interconnect is installed. EPSRC are also reviewing allocation models.
- Low Priority Access accounted for 4.6% of the XT4 utilisation, and 46.7% of the XT6 utilisation in 3Q10. This initiative will remain in force until the arrival of Gemini.
- The service was far more reliable in 3Q10 than in the previous quarter. There were 7 service failures in 3Q10 as opposed to 16 in 2Q10. 6 failures were attributed to technology problems and there was one external security failure. The overall MTBF increased on 2Q10 from 137 to 366 hours.
- The performance metrics in 3Q10 were excellent. Reliability, Technology MTBF and the Capability Job Completion Rate all exceeded the full service level.
- The volume of single node failures has remained constant from the previous quarter.
- The helpdesk statistics were again excellent. No negative quality tokens were received from users in 3Q10 and a number of positive tokens were received.
- The X2 Vector system was very reliable in 3Q10. Charging remained suspended on the X2, resulting in an overall utilisation of 48.1%, compared to 39.9% in 2Q10. Further details on X2 utilisation are available in Section 3.2.5.
- The installation of the external lustre filesystem in 3Q10 did not go ahead as planned. A number of additional issues were encountered. The migration of user data to esFS has now been postponed until October 2010 pending the results of a 10-day dedicated testing and debugging period. Details are available in Section 5.1.1.
- The upgrade to the Gemini interconnect is now expected to take place in January 2011.
- A HECToR User Group meeting took place on October 12th. A number of options for HECToR Phase3 were presented.

3 Quantitative Metrics

3.1 Reliability

The metrics in Section 3.1 relate solely to the service machine – i.e. Phase 2a.

The monthly numbers of incidents and failures (SEV 1 incidents) are shown in the table below:

| | Jul | Aug | Sep |
|-----------|-----|-----|-----|
| Incidents | 17 | 25 | 26 |
| Failures | 3 | 2 | 2 |

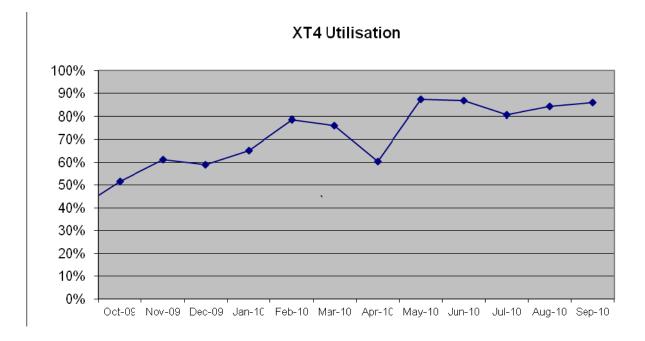
3.1.1 Performance Statistics

MTBF = (732)/(number of failures in a month)
Quarterly MTBF=(3x732)/(number of failures in a quarter)

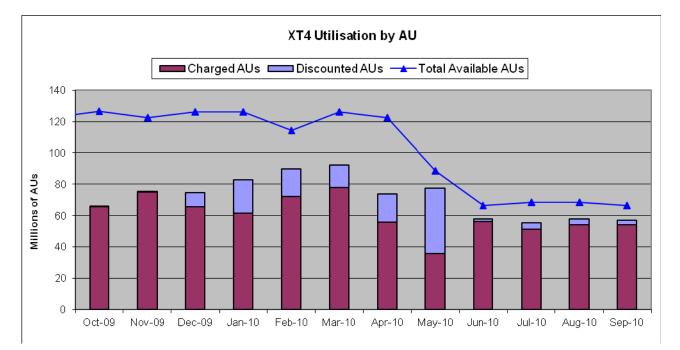
| Attribution | Metric | Jul | Aug | Sep | Quarterly |
|----------------------|----------|-----|-----|-----|-----------|
| Technology | Failures | 3 | 2 | 1 | 6 |
| rechnology | MTBF | 244 | 366 | 732 | 366 |
| Service Provision | Failures | 0 | 0 | 0 | 0 |
| | MTBF | 8 | ∞ | ∞ | 8 |
| External | Failures | 0 | 0 | 1 | 1 |
| | MTBF | ∞ | ∞ | 732 | 2196 |
| Overall | Failures | 3 | 2 | 2 | 7 |
| | MTBF | 244 | 366 | 366 | 314 |

3.2 HECToR Utilisation

3.2.1 XT4 Utilisation



The XT4 utilisation quarterly average in 3Q10 was 83.6%, compared to 75% in 2Q10.

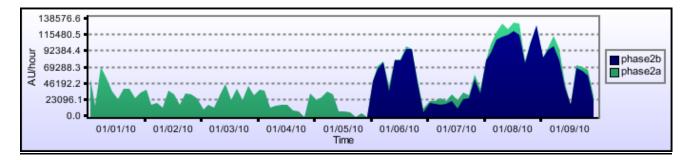


Capability Incentives

Capability incentive levels were reviewed in 3Q10 and the same discount rates now apply on both the Phase 2a And Phase 2b machines.

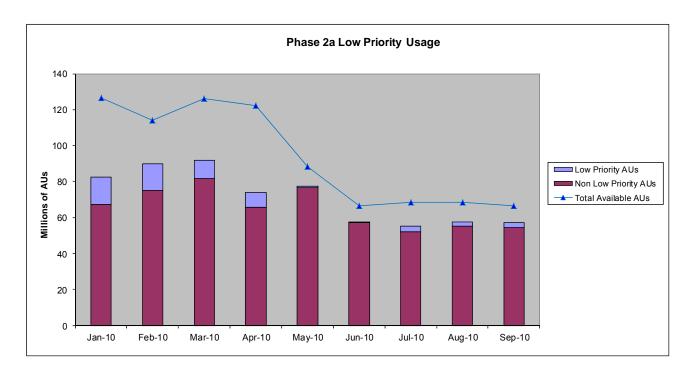
| Level | Minimum Number of Cores | Discount |
|--------|-------------------------|----------|
| Bronze | 2048 | 5% |
| Silver | 4096 | 15% |
| Gold | 8192 | 30% |

As can be seen below, the introduction of the Phase 2b system has clearly increased the capability for running large jobs.

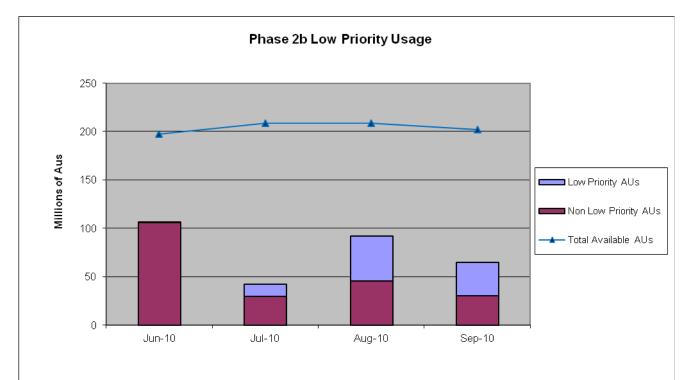


Low Priority Access

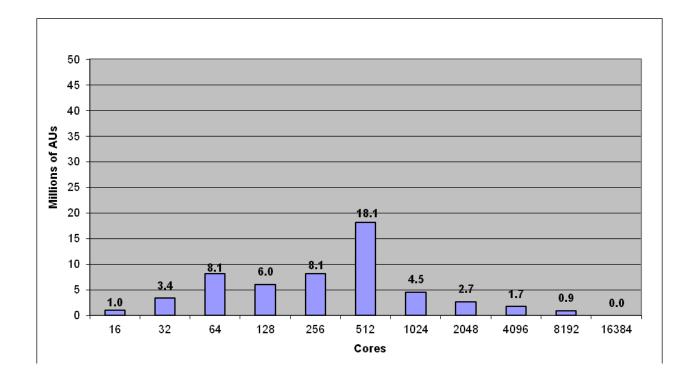
In 3Q10, low priority access accounted for 4.6% of the overall utilisation on the XT4. It continues to fill the available gaps.



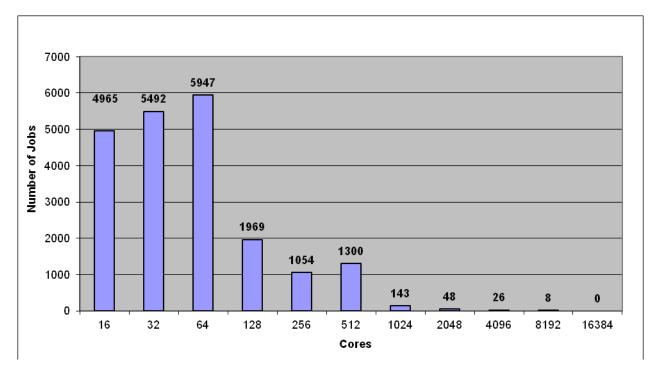
In 3Q10, low priority access accounted for 46.7% of the overall utilisation on the XT6.



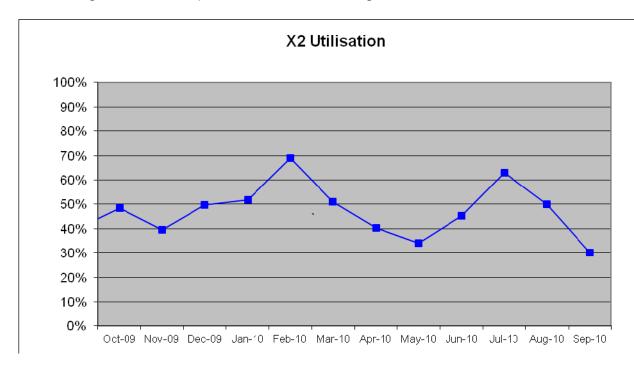
3.2.2 XT4 Utilisation by Core Count



3.2.3 XT4 Number of jobs by Core Count



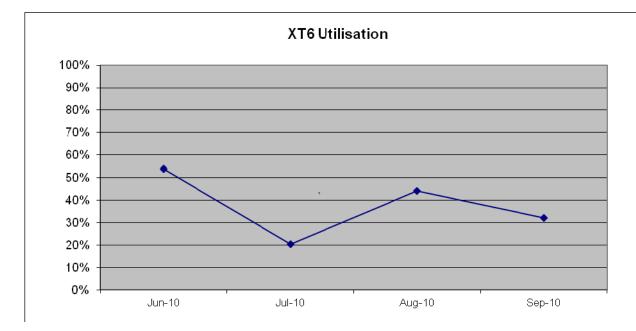
3.2.5 X2 Utilisation



Accounting remained suspended on the X2 throughout 3Q10.

The overall X2 utilisation for 3Q10 was 48.1%. We have contacted all of the key users of the X2 to understand what their requirement would be for maintaining the X2 capability beyond Phase 2 of the service. The feedback will be collated and passed to the research councils.

3.2.6 XT6 Utilisation



Utilisation on the XT6 remains lower than we would like.

Charging was initially suspended during the availability trial phase of the upgrade. The trial completed successfully on 24th June, and charging was enabled on 28th June. The Linpack based AU rate was initially discounted by an agreed 20% in order to allow for any performance impact whilst we await the Gemini interconnect. This discount was later reviewed and was increased to 40% as of 29th September.

Despite the low utilisation percentage figure, it is worth noting that in 3Q10 more AUs were used on the XT6 than on the XT4. There is now a far greater capacity on the service. The challenge is to grow the use of the service to match the increased capacity.

3.2.4 Utilisation by Consortium

| Project | XT4 Utilisation | XT6 Utilisation | X2 Utilisation |
|----------------|-----------------|-----------------|----------------|
| y01 | 0.0% | 0.0% | 0.0% |
| y02 | 0.0% | 0.3% | 0.0% |
| y03 | 0.0% | 0.0% | 0.0% |
| y04 | 0.0% | 0.0% | 0.0% |
| y05 | 0.0% | 0.0% | 0.0% |
| y06 | 0.0% | 0.0% | 0.0% |
| y07 | 0.0% | 0.0% | 0.0% |
| z01 | 0.1% | 0.0% | 0.0% |
| z02 | 0.0% | 0.0% | 0.0% |
| z03 | 0.0% | 0.2% | 0.0% |
| z06 | 0.0% | 0.0% | 0.0% |
| Internal Total | 0.1% | 0.5% | 0.0% |
| c01 | 1.6% | 0.2% | 0.0% |
| e01 | 3.6% | 7.2% | 45.1% |
| e05 | 7.0% | 1.5% | 2.6% |
| e10 | 0.1% | 0.0% | 0.0% |
| e24 | 10.8% | 2.9% | 0.0% |
| e35 | 0.0% | 0.0% | 0.0% |
| e42 | 0.0% | 0.0% | 0.0% |
| e59 | 0.0% | 0.0% | 0.0% |
| e63 | 1.3% | 0.1% | 0.0% |
| e68 | 0.9% | 0.3% | 0.0% |
| e71 | 0.6% | 0.0% | 0.0% |
| e75 | 0.0% | 0.0% | 0.0% |
| e76 | 1.3% | 0.0% | 0.0% |
| e81 | 0.0% | 0.0% | 0.0% |
| e82 | 0.0% | 0.0% | 0.0% |
| e84 | 0.1% | 0.0% | 0.0% |
| e85 | 0.0% | 0.5% | 0.0% |
| e89 | 6.7% | 7.3% | 0.0% |
| e92 | 0.0% | 0.1% | 0.0% |
| e102 | 0.1% | 0.0% | 0.0% |
| e104 | 0.2% | 0.0% | 0.0% |
| e107 | 0.0% | 0.0% | 0.0% |
| e110 | 1.4% | 1.0% | 0.0% |
| e113 | 0.0% | 0.0% | 0.0% |
| e117 | 3.7% | 0.0% | 0.0% |
| e120 | 0.0% | 0.0% | 0.0% |
| e121 | 2.2% | 0.0% | 0.0% |
| e122 | 1.3% | 0.1% | 0.0% |
| e124 | 0.0% | 0.6% | 0.0% |
| e125 | 0.7% | 1.2% | 0.0% |
| e126 | 0.5% | 0.0% | 0.0% |
| e127 | 0.0% | 0.0% | 0.0% |
| e129 | 0.1% | 0.0% | 0.0% |
| e131 | 0.0% | 0.0% | 0.0% |
| e132 | 0.0% | 0.0% | 0.0% |
| e136 | 1.3% | 0.0% | 0.0% |
| e137 | 0.0% | 0.0% | 0.0% |
| e138 | 0.0% | 0.0% | 0.0% |

| Project | XT4 Utilisation | XT6 Utilisation | X2 Utilisation |
|----------------------|-----------------|-----------------|----------------|
| e139 | 0.0% | 0.0% | 0.0% |
| e141 | 0.0% | 0.4% | 0.0% |
| e144 | 0.0% | 0.0% | 0.0% |
| e145 | 0.0% | 0.0% | 0.0% |
| e147 | 0.0% | 0.0% | 0.0% |
| e148 | 0.0% | 0.0% | 0.0% |
| e149 | 1.0% | 0.0% | 0.0% |
| e150 | 0.2% | 0.0% | 0.0% |
| e151 | 0.3% | 0.1% | 0.0% |
| e152 | 0.1% | 2.3% | 0.0% |
| e153 | 0.0% | 0.0% | 0.0% |
| e154 | 1.0% | 0.0% | 0.0% |
| e156 | 0.0% | 0.0% | 0.0% |
| e157 | 0.0% | 0.0% | 0.0% |
| e162 | 0.0% | 0.0% | 0.0% |
| e163 | 0.2% | 0.0% | 0.0% |
| e167 | 0.0% | 0.0% | 0.0% |
| e169 | 0.0% | 0.0% | 0.0% |
| e171 | 0.3% | 0.0% | 0.0% |
| e172 | 0.2% | 0.0% | 0.0% |
| e173 | 0.0% | 0.0% | 0.0% |
| e174 | 0.2% | 0.0% | 0.0% |
| EPSRC Total | 49.4% | 26.1% | 47.7% |
| e178 | 0.0% | 0.0% | 0.0% |
| n01 | 4.4% | 1.5% | 0.0% |
| n02 | 17.9% | 1.7% | 0.0% |
| n03 | 9.0% | 0.7% | 0.0% |
| n04 | 1.6% | 1.0% | 0.0% |
| NERC Total | 32.9% | 4.9% | 0.0% |
| b09 | 0.0% | 0.2% | 0.0% |
| b10 | 0.0% | 0.0% | 0.0% |
| b100 | 0.1% | 0.0% | 0.0% |
| BBSRC Total | 0.1% | 0.3% | 0.0% |
| p01 | 0.0% | 0.0% | 0.0% |
| STFC Total | 0.0% | 0.0% | 0.0% |
| e168 | 0.0% | 0.0% | 0.0% |
| t01 | 0.6% | 0.0% | 0.0% |
| x01 | 0.3% | 0.2% | 0.0% |
| x05 | 0.1% | 0.0% | 0.0% |
| x06 | 0.0% | 0.0% | 0.0% |
| External Total | 1.0% | 0.2% | 0.0% |
| d03 | 0.0% | 0.0% | 0.0% |
| d04 | 0.0% | 0.0% | 0.0% |
| d11 | 0.0% | 0.0% | 0.0% |
| d14 | 0.0% | 0.1% | 0.0% |
| d16 | 0.0% | 0.0% | 0.0% |
| d17 | 0.0% | 0.0% | 0.3% |
| d18 | 0.0% | 0.0% | 0.0% |
| d19 | 0.0% | 0.0% | 0.0% |
| d22 | 0.0% | 0.0% | 0.0% |
| d23 | 0.0% | 0.0% | 0.0% |
| Directors Time Total | 0.0% | 0.2% | 0.3% |
| Overall Total | 83.6% | 32.2% | 48.1% |

3.3. Performance Metrics

| Metric | TSL(%) | FSL(%) | Jul-10 | Aug-10 | Sep-10 | 3Q10 |
|--|--------|--------|--------|--------|--------|--------|
| Technology reliability (%) | 85.00% | 98.50% | 99.3% | 98.6% | 99.9% | 99.2% |
| Technology MTBF (hours) | 100 | 126.4 | 244.0 | 366.0 | 366.0 | 366.0 |
| Technology Throughput, hours/year | 7000 | 8367 | 8601 | 8348 | 8307 | 8418 |
| Capability jobs completion rate | 70% | 90% | 97.7% | 98.2% | 96.7% | 97.2% |
| Non in-depth queries resolved within 1 day (%) | 85% | 97% | 100.0% | 99.0% | 97.7% | 98.9% |
| Number of SP FTEs | 7.3 | 8.0 | 9.0 | 9.0 | 9.1 | 9.0 |
| SP Serviceability (%) | 80.00% | 99.00% | 100.0% | 100.0% | 100.0% | 100.0% |

All performance metrics relate solely to the service machine – i.e. Phase 2a.

Colour coding:

| Exceeds FSL | |
|---------------------|--|
| Between TSL and FSL | |
| Below TSL | |

The performance metrics in 3Q10 were excellent. Reliability, Technology MTBF and the Capability Job Completion Rate all exceeded the full service level.

4. Helpdesk

A total of 902 queries with a specified service metric were completed in this period.

Helpdesk Targets

| Metric | Pass | Total | Fraction | Target |
|----------------------------------|------|-------|----------|--------|
| All queries finished in 1 day | 739 | 746 | 99.1% | 97.0% |
| Admin queries finished in 1 day | 668 | 674 | 99.1% | 97.0% |
| Queries assigned in 30 min | 891 | 891 | 100.0% | 97.0% |
| Technical assessments in 10 days | 35 | 35 | 100% | 97.0% |

Queries by Service Metric

| Service Metric | Queries | Percentage |
|------------------------------|---------|------------|
| Automatic | 474 | 52.55% |
| Admin | 200 | 22.17% |
| In-depth | 121 | 13.41% |
| Technical | 72 | 7.98% |
| Technical assessment class-1 | 28 | 3.10% |
| Technical assessment class-2 | 7 | 0.78% |

Queries by Category

| Query Category | Queries | Percentage |
|-------------------------------|---------|------------|
| New User | 125 | 13.90% |
| Set group quotas | 100 | 11.10% |
| New Password | 81 | 9.00% |
| None | 66 | 7.30% |
| 3rd Party Software | 65 | 7.20% |
| Access to HECToR | 62 | 6.90% |
| User behaviour | 47 | 5.20% |
| Set user quotas | 44 | 4.90% |
| Disk, tapes, resources | 42 | 4.70% |
| Add to group | 36 | 4.00% |
| Batch system and queues | 26 | 2.90% |
| New Group | 24 | 2.70% |
| Join Project | 23 | 2.50% |
| Compilers and system software | 23 | 2.50% |
| Node Failure | 20 | 2.20% |
| User programs | 19 | 2.10% |
| Login, passwords and ssh | 14 | 1.60% |
| Update account | 13 | 1.40% |
| Other | 13 | 1.40% |
| Remove account | 11 | 1.20% |
| SAFE | 10 | 1.10% |
| Delete from group | 10 | 1.10% |
| Archive | 9 | 1.00% |

| Courses | 6 | 0.70% |
|-------------------------|---|-------|
| Static website | 3 | 0.30% |
| Delete from project | 3 | 0.30% |
| Create certificate | 3 | 0.30% |
| Performance and scaling | 2 | 0.20% |
| Porting | 1 | 0.10% |
| Network | 1 | 0.10% |

Queries by Handler Category

| Handlers | Total | Automatic | Technical Assessment | Admin | Technical | In- depth | %age |
|----------|-------|-----------|-------------------------|-------|-----------|--------------|--------|
| OSG | 517 | 473 | | 15 | 24 | 5 | 57.32% |
| CSE | 91 | | 35 | | 1 | 55 | 10.09% |
| USL | 261 | 1 | | 185 | 37 | 38 | 28.94% |
| Cray | 33 | | | | 10 | 23 | 3.66% |

4.1 Quality Tokens

A number of positive quality tokens were set by users during 3Q10. No negative tokens were received.

| Project | Negative Tokens | Positive Tokens |
|---------|-----------------|-----------------|
| e125 | 0 | 5 |
| e89 | 0 | 5 |
| Total | 0 | 10 |

5 System Hardware

5.1 HECToR Technology Changes

5.1.1 esFS Upgrade

The migration to external <u>lustre (esFS)</u> was originally planned for 2Q10. Due to the major issues encountered in April, this was then delayed until 3Q10. Further issues with the upgrade were then encountered in July and August and the planned migration of user data was postponed for a second time. The decision was taken in late September to remove the Phase 2a system from user service in October for a period of 10-days to enable dedicated testing and debugging to take place. The migration of user data will commence thereafter.

5.1.2 CLE3.1 Upgrade

The operating system on the Phase 2b service was upgraded on 29th September. All core third party applications, including the Unified Model were tested prior to the upgrade, and no major issues were encountered.

5.1.3 Gemini Upgrade

The upgrade to the Gemini interconnect has been delayed until the migration to esFS is complete. This is now expected to take place in January 2011.

5.2 Severity-1 Incidents

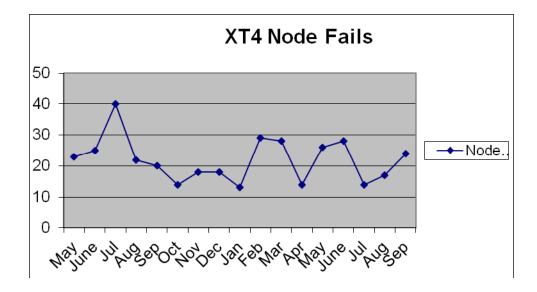
The monthly numbers of incidents and failures (SEV 1 incidents) are shown in the table below:

| | Jul | Aug | Sep |
|-----------|-----|-----|-----|
| Incidents | 17 | 25 | 26 |
| Failures | 3 | 2 | 2 |

Technology failures were responsible for 6 of the Severity-1 incidents during 3Q10. Of the 6 technology failures, there was no particular trend. There was one process failure among them, and the other 5 failures were distinct hardware faults. In addition, there was one external security alert. There were no service provision failures in 3Q10.

5.3 Single Node Failures

Node failure rates as a result of DIMM failures and Opteron Cache failures remain very low. Most node failures on the XT4 relate to communications errors



On the XT6 system, node failure rates are also low. The majority of errors relate to an 'Out of Memory' software condition. This is an issue which is fixed in CLE3.1 and which was installed on the XT6 on 29th September.

Appendix A: Terminology

| TSL | : | Threshold Service Level |
|--------|---------|---|
| FSL | : | Full Service Level |
| SDT | : | Scheduled Down Time |
| UDT | : | Unscheduled Down Time |
| WCT | : | Wall Clock Time |
| MTBF | : | Mean Time Between Failures = 732/Number of Failures |
| SP | : | Service Provision |
| SP Ser | viceabi | lity% = 100*(WCT-SDT-UDT(SP))/(WCT-SDT) |
| | | |

Technology Reliability % = 100*(1-(UDT(Technology)/(WCT-SDT))

Incident Severity Levels

SEV 1 — anything that comprises a FAILURE as defined in the contract with EPSRC.

SEV 2 — NON-FATAL incidents that typically cause immediate termination of a user application, but not the entire user service.

The service may be so degraded (or liable to collapse completely) that a controlled, but unplanned (and often very short-notice) shutdown is required or unplanned downtime subsequent to the next planned reload is necessary.

This category includes unrecovered disc errors where damage to file systems may occur if the service was allowed to continue in operation; incidents when although the service can continue in operation in a degraded state until the next reload, downtime at less than 24 hours notice is required to fix or investigate the problem; and incidents whereby the throughput of user work is affected (typically by the unrecovered disabling of a portion of the system) even though no subsequent unplanned downtime results.

SEV 3 — NON-FATAL incidents that typically cause immediate termination of a user application, but the service is able to continue in operation until the next planned reload or re-configuration.

SEV 4 — NON-FATAL recoverable incidents that typically include the loss of a storage device, or a peripheral component, but the service is able to continue in operation largely unaffected, and typically the component may be replaced without any future loss of service.

Appendix B: Projects on HECToR

| Code | Title | Funding Body | Class | PI | Total AUs allocated | AUs used | AUs left |
|-------|---|-----------------|---------|-----------------------------|---------------------|-------------|---------------|
| EPSRC | Projects | | | | | | |
| e01 | UK Turbulence Consortium | EPSRC | Class1a | Dr Gary N Coleman | 483,969,876 | 26,143,639 | 457,826,237 |
| e05 | Materials Chemistry HPC Consortium | EPSRC | Class1a | Prof C Richard A Catlow | 1,139,124,000 | 100,979,241 | 1,038,084,759 |
| e10 | GENIUS | EPSRC | Class1a | Prof Peter Coveney | 10,248,188 | 6,572,530 | 3,675,658 |
| e101 | Optimization of HPCx LES code | EPSRC | Class2a | Prof Michael Leschziner | 641,009 | 642,368 | -1,359 |
| e104 | Fluid-Mechanical Models applied to Heart Failure | EPSRC | Class1a | Dr Nicolas Smiths | 30,400,000 | 852,477 | 29,547,523 |
| e105 | Joint Euler/Lagrange Method for Multi- Scale Problems | EPSRC | Class1a | Dr Andreas M Kempf | 1,300,000 | 297,323 | 1,002,677 |
| e106 | Numerical Simulation of Multiphase Flow: From Mesocales to | EPSRC | Class1a | Prof Kai Luo | 3,650,000 | 0 | 3,650,000 |
| e107 | Parallel Brain Surgery Simulation | EPSRC | Class1a | Dr Stephane P. A. Bordas | 6,000,000 | 332,482 | 5,667,518 |
| e108 | Unsteady Propeller Noise | EPSRC | Class2b | Dr Sergey Karabasov | 673,164 | 158,100 | 515,064 |
| e110 | Computational Aeroacoustics Consortium | EPSRC | Class1a | Prof Paul Tucker | 39,100,000 | 25,440,934 | 13,659,066 |
| e117 | Binding free energy estimations | EPSRC | Class1b | Dr Carmen Domene | 12,247,664 | 12,289,068 | -41,404 |
| e122 | Multiscale Modelling of Magnetised Plasma Turbulence | EPSRC | Class1a | Dr Colin M Roach | 65,000,000 | 18,539,258 | 46,460,742 |
| e124 | Compressible Axisymmetric Flows | EPSRC | Class1a | Dr Richard D Sandberg | 22,887,943 | 5,885,963 | 17,001,980 |
| e125 | Full configuration interaction quantum monte carlo | EPSRC | Class1a | Dr Ali Alavi | 18,324,825 | 3,572,645 | 14,752,180 |
| e126 | Clean Coal Combustion: Burning Issues of Syngas Burning | EPSRC | Class1a | Prof Xi Jiang | 9,984,000 | 4,213,941 | 5,770,059 |

| Title | Funding Body | Class | PI | Total AUs allocated | AUs used | AUs left |
|--|--|--|---|---|--|---|
| Alternative drag-reduction strategies | EPSRC | Class1a | Prof Michael Leschziner | 7,000,000 | 2,852 | 6,997,148 |
| Rate-Controlled Constrained Equilibrium | EPSRC | Class1a | Dr Stelios Rigopoulos | 6,230,000 | 0 | 6,230,000 |
| Novel Hybrid LES-RANS schemes [ICL] | EPSRC | Class1a | Prof Michael Leschziner | 7,500,000 | 263,821 | 7,236,179 |
| Novel hybrid LES-RANS schemes [MAN] | EPSRC | Class1a | Prof Dominique Laurence | 10,500,000 | 0 | 10,500,000 |
| Direct Simulation of a Pure Plume impinging on a density surface | EPSRC | Class2a | Dr Maarten van Reeuwijk | 265,000 | 76,896 | 188,104 |
| Implementation of Established Algorithms to Extend HELIUM | EPSRC | Class2b | Prof Ken Taylor | 800,000 | 0 | 800,000 |
| Numerical Simulation of Turbomachinery Flows | EPSRC | Class2a | Dr Francesco Montomoli | 291,790 | 16,419 | 275,371 |
| Modelling the UK Wind Power Resource | EPSRC | Class1b | Dr Gareth Harrison | 5,679,268 | 3,503,388 | 2,175,880 |
| Turbulent Pipe Flow | EPSRC | Class2a | Prof Dwight Barkley | 200,000 | 205,320 | -5,320 |
| A numerical study of turbulent manoeuvering-body wakes | EPSRC | Class1a | Dr Gary N Coleman | 16,350,000 | 144,332 | 16,205,668 |
| Numerical Simulation of Rotating Stall and Surge | EPSRC | Class1a | Dr Mehdi Vahdati | 1,266,001 | 24 | 1,265,977 |
| UK-SHEC Consortium | EPSRC | Class1a | Dr T.J. Mays | 1,191,899 | 182,408 | 1,009,491 |
| Scale adaptive simulations of turbulent flows | EPSRC | Class2a | Prof Oubay Hassan | 243,495 | 130,309 | 113,186 |
| Adding the molecular dynamics functionality to the quantum | EPSRC | Class2b | Prof Dario Alfe` | 638,951 | 263,691 | 375,260 |
| Fractal-generated turbulence and mixing: flow physics and | EPSRC | Class1a | Prof Christos Vassilicos | 51,920,000 | 2,620,215 | 49,299,785 |
| Modelling Cholesterol Deposits | EPSRC | Class1a | Dr David Quigley | 10,000,000 | 0 | 10,000,000 |
| Metal Conquest: efficient simulation of metals on petaflop | EPSRC | Class2b | Dr David Bowler | 800,000 | 212 | 799,788 |
| Global stability computations of separated flows | EPSRC | Class2a | Prof Jitesh S B Gajjar | 299,996 | 98 | 299,898 |
| | Alternative drag-reduction strategies Rate-Controlled Constrained Equilibrium Novel Hybrid LES-RANS schemes [ICL] Novel hybrid LES-RANS schemes [MAN] Direct Simulation of a Pure Plume impinging on a density surface Implementation of Established Algorithms to Extend HELIUM Numerical Simulation of Turbomachinery Flows Modelling the UK Wind Power Resource Turbulent Pipe Flow A numerical study of turbulent manoeuvering-body wakes Numerical Simulation of Rotating Stall and Surge UK-SHEC Consortium Scale adaptive simulations of turbulent flows Adding the molecular dynamics functionality to the quantum Fractal-generated turbulence and mixing: flow physics and Modelling Cholesterol Deposits Metal Conquest: efficient simulation of metals on petaflop Global stability computations of separated | InteBodyAlternative drag-reduction strategiesEPSRCRate-Controlled Constrained EquilibriumEPSRCNovel Hybrid LES-RANS schemes [ICL]EPSRCNovel hybrid LES-RANS schemes [MAN]EPSRCDirect Simulation of a Pure Plume impinging on a density surfaceEPSRCImplementation of Established Algorithms to Extend HELIUMEPSRCNumerical Simulation of Turbomachinery FlowsEPSRCModelling the UK Wind Power ResourceEPSRCTurbulent Pipe FlowEPSRCA numerical study of turbulent manoeuvering-body wakesEPSRCNumerical Simulation of Rotating Stall and SurgeEPSRCUK-SHEC ConsortiumEPSRCScale adaptive simulations of turbulent flowsEPSRCAdding the molecular dynamics functionality to the quantumEPSRCFractal-generated turbulence and mixing: flow physics andEPSRCModelling Cholesterol DepositsEPSRCMetal Conquest: efficient simulation of metals on petaflopEPSRCGlobal stability computations of separated EPSRCEPSRC | InteBodyClassAlternative drag-reduction strategiesEPSRCClass1aRate-Controlled Constrained EquilibriumEPSRCClass1aNovel Hybrid LES-RANS schemes [ICL]EPSRCClass1aNovel hybrid LES-RANS schemes [MAN]EPSRCClass1aDirect Simulation of a Pure Plume impinging on a density surfaceEPSRCClass2aImplementation of Established Algorithms to Extend HELIUMEPSRCClass2aNumerical Simulation of Turbomachinery FlowsEPSRCClass2aModelling the UK Wind Power ResourceEPSRCClass1aTurbulent Pipe FlowEPSRCClass1aNumerical study of turbulent manoeuvering-body wakesEPSRCClass1aUK-SHEC ConsortiumEPSRCClass1aScale adaptive simulations of turbulent flowsEPSRCClass2aAdding the molecular dynamics functionality to the quantumEPSRCClass1aFractal-generated turbulence and mixing: flow physics andEPSRCClass1aModelling Cholesterol DepositsEPSRCClass1aMetal Conquest: efficient simulation of metals on petaflopEPSRCClass2aGlobal stability computations of separated Global stability computations of separatedEPSRCClass2a | InteBodyClassP1Alternative drag-reduction strategiesEPSRCClass1aProf Michael LeschzinerRate-Controlled Constrained EquilibriumEPSRCClass1aDr Stelios RigopoulosNovel Hybrid LES-RANS schemes [ICL]EPSRCClass1aProf Michael LeschzinerNovel hybrid LES-RANS schemes [MAN]EPSRCClass1aProf Dominique LaurenceDirect Simulation of a Pure Plume impinging on a density surfaceEPSRCClass2aDr Maarten van ReeuwijkImplementation of Established Algorithms to Extend HELIUMEPSRCClass2aDr Francesco MontomoliNumerical Simulation of Turbomachinery FlowsEPSRCClass1aDr Francesco MontomoliModelling the UK Wind Power ResourceEPSRCClass1aDr Gareth HarrisonTurbulent Pipe FlowEPSRCClass1aDr Gary N Coleman Numerical Simulation of Rotating Stall and SurgeEPSRCClass1aDr Gary N ColemanNumerical Simulation of Rotating Stall and SurgeEPSRCClass1aDr T.J. MaysScale adaptive simulations of turbulent flowsEPSRCClass1aDr T.J. MaysScale adaptive simulations of turbulent flowsEPSRCClass1aProf Dario Alfe'Fractal-generated turbulence and mixing: flow physics andEPSRCClass1aDr Christos VassilicosModelling Cholesterol DepositsEPSRCClass1aDr David QuigleyMetal Conquest: efficient simulation of metals on petaflopEPSRCClass2aProf Ditesh S B <td>InteBodyClassP1allocatedAlternative drag-reduction strategiesEPSRCClass1aProf Michael Leschziner7,000,000Rate-Controlled Constrained EquilibriumEPSRCClass1aDr Stelios Rigopoulos6,230,000Novel Hybrid LES-RANS schemes [ICL]EPSRCClass1aProf Michael Leschziner7,500,000Novel Hybrid LES-RANS schemes [ICL]EPSRCClass1aProf Michael Leschziner7,500,000Direct Simulation of a Pure Plume impinging on a density surfaceEPSRCClass2aDr Maarten van Reeuwijk265,000Implementation of Established Algorithms to Extend HELUMEPSRCClass2aDr Francesco Mortomoli291,790Nodelling the UK Wind Power ResourceEPSRCClass2aDr Gareth Harrison5,679,268Turbulent Pipe FlowEPSRCClass1aDr Gary N Coleman16,350,000A numerical study of turbulent maneeuvering-body wakesEPSRCClass1aDr Gary N Coleman16,350,000Numerical Simulation of Rotating Stall and SurgeEPSRCClass1aDr Gary N Coleman16,350,000UK-SHEC ConsortiumEPSRCClass1aDr Mehdi Vahdati1,266,001UK-SHEC ConsortiumEPSRCClass1aDr Gory N Coleman16,350,000Numerical Simulation of Rotating Stall and SurgeEPSRCClass1aDr Gary N Coleman16,350,000Numerical simulation of notating Stall and SurgeEPSRCClass1aDr Gory N Coleman16,350,000Modelling the molecular dy</td> <td>InteBodyClassP1allocatedAdvs usedAlternative drag-reduction strategiesEPSRCClass1aProf Michael Leschziner7,000,0002,852Rate-Controlled Constrained EquilibriumEPSRCClass1aDr Stellos6,230,0000Novel Hybrid LES-RANS schemes [ICL]EPSRCClass1aProf Michael Leschziner7,500,000263,821Novel Hybrid LES-RANS schemes [MAN]EPSRCClass1aProf Michael Leschziner7,500,0000Direct Simulation of a Pure Plume impinging on a density surfaceEPSRCClass2aReewijk265,00076,896Implementation of Established Algorithms to Extend HELIUMEPSRCClass2aProf Ken Taylor800,00000Numerical Simulation of Turbomachinery FlowsEPSRCClass2aProf Dwinique Laurence291,79016,419Modelling the UK Wind Power ResourceEPSRCClass2aProf Dwinght Barkley200,000205,320A numerical study of turbulent maneeuvering-body wakesEPSRCClass1aDr Gary N Coleman16,350,000144,332Numerical Simulation of Rotating Stall and SurgeEPSRCClass1aDr Gary N Coleman16,350,000244UK-SHEC ConsortiumEPSRCClass1aDr J. 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Mays1,19</td> | InteBodyClassP1allocatedAlternative drag-reduction strategiesEPSRCClass1aProf Michael Leschziner7,000,000Rate-Controlled Constrained EquilibriumEPSRCClass1aDr Stelios Rigopoulos6,230,000Novel Hybrid LES-RANS schemes [ICL]EPSRCClass1aProf Michael Leschziner7,500,000Novel Hybrid LES-RANS schemes [ICL]EPSRCClass1aProf Michael Leschziner7,500,000Direct Simulation of a Pure Plume impinging on a density surfaceEPSRCClass2aDr Maarten van Reeuwijk265,000Implementation of Established Algorithms to Extend HELUMEPSRCClass2aDr Francesco Mortomoli291,790Nodelling the UK Wind Power ResourceEPSRCClass2aDr Gareth Harrison5,679,268Turbulent Pipe FlowEPSRCClass1aDr Gary N Coleman16,350,000A numerical study of turbulent maneeuvering-body wakesEPSRCClass1aDr Gary N Coleman16,350,000Numerical Simulation of Rotating Stall and SurgeEPSRCClass1aDr Gary N Coleman16,350,000UK-SHEC ConsortiumEPSRCClass1aDr Mehdi Vahdati1,266,001UK-SHEC ConsortiumEPSRCClass1aDr Gory N Coleman16,350,000Numerical Simulation of Rotating Stall and SurgeEPSRCClass1aDr Gary N Coleman16,350,000Numerical simulation of notating Stall and SurgeEPSRCClass1aDr Gory N Coleman16,350,000Modelling the molecular dy | InteBodyClassP1allocatedAdvs usedAlternative drag-reduction strategiesEPSRCClass1aProf Michael Leschziner7,000,0002,852Rate-Controlled Constrained EquilibriumEPSRCClass1aDr Stellos6,230,0000Novel Hybrid LES-RANS schemes [ICL]EPSRCClass1aProf Michael Leschziner7,500,000263,821Novel Hybrid LES-RANS schemes [MAN]EPSRCClass1aProf Michael Leschziner7,500,0000Direct Simulation of a Pure Plume impinging on a density surfaceEPSRCClass2aReewijk265,00076,896Implementation of Established Algorithms to Extend HELIUMEPSRCClass2aProf Ken Taylor800,00000Numerical Simulation of Turbomachinery FlowsEPSRCClass2aProf Dwinique Laurence291,79016,419Modelling the UK Wind Power ResourceEPSRCClass2aProf Dwinght Barkley200,000205,320A numerical study of turbulent maneeuvering-body wakesEPSRCClass1aDr Gary N Coleman16,350,000144,332Numerical Simulation of Rotating Stall and SurgeEPSRCClass1aDr Gary N Coleman16,350,000244UK-SHEC ConsortiumEPSRCClass1aDr J. 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| Title | Funding Body | Class | PI | Total AUs allocated | AUs used | AUs left |
|---|---|--|--|---|---|--|
| Novel Asynchronous Algorithms | EPSRC | Class1a | Prof Nicholas J Higham | 500,000 | 0 | 500,000 |
| Multi-layered Abstractions for PDEs | EPSRC | Class1a | Prof Paul Kelly | 3,816,000 | 0 | 3,816,000 |
| Sustainable Software Generation Tools | EPSRC | Class1a | Prof Paul Kelly | 20,208,060 | 0 | 20,208,060 |
| Properties and Dynamics of Atomic Bose- Einstein Condensates | EPSRC | Class1a | Dr A White | 69,895,466 | 0 | 69,895,466 |
| Multi-scale simulation of intense laser plasma interactions | EPSRC | Class1a | Dr Tony Arber | 4,872,000 | 0 | 4,872,000 |
| Large Eddy Simulation of LNG Pool Fires | EPSRC | Class2a | Dr Siaka Dembele | 300,000 | 82,964 | 217,036 |
| LES of supersonic jets | EPSRC | Class1b | Prof William Dawes | 2,696,000 | 155,781 | 2,540,219 |
| Conformational switching of tetra- (bromophenyl) porphyrins | EPSRC | Class1b | Prof Mats Persson | 1,704,960 | 1,734,321 | -29,361 |
| Performance of oomph-lib in largescale parallel computations | EPSRC | Class2a | Prof Matthias Heil | 300,000 | 44,139 | 255,861 |
| 3D instabilities in two-layer flows | EPSRC | Class2a | Dr Prashant Valluri | 701,899 | 401,899 | 300,000 |
| Structure refinement of nanomaterials | EPSRC | Class2a | Prof. Peter G Bruce | 300,000 | 0 | 300,000 |
| Amorphous structures of mirror coatings | EPSRC | Class2a | Dr Ian Maclaren | 300,000 | 0 | 300,000 |
| Edinburgh Soft Matter and Statistical Physics Group | EPSRC | Class1a | Prof Michael Cates | 4,663 | 6,171 | -1,508 |
| DEISA | EPSRC | Class1a | Mrs Alison Kennedy | 233,146,943 | 115,245,818 | 117,901,125 |
| UK Applied Aerodynamics Consortium 2 | EPSRC | Class1a | Dr Nick Hills | 30,925,323 | 20,468,761 | 10,456,562 |
| Hydrogenation Reactions at Metal Surfaces | EPSRC | Class1a | Prof. Angelos Michaelides | 50,000,000 | 41,243,007 | 8,756,993 |
| Simulating the control of calcite crystallisation | EPSRC | Class1a | Prof John Harding | 130,403,522 | 41,413,263 | 88,990,259 |
| HELIUM Developments | EPSRC | Class1a | Prof Ken Taylor | 42,521,798 | 33,211,189 | 9,310,609 |
| | Multi-layered Abstractions for PDEs Sustainable Software Generation Tools Properties and Dynamics of Atomic Bose- Einstein Condensates Multi-scale simulation of intense laser plasma interactions Large Eddy Simulation of LNG Pool Fires LES of supersonic jets Conformational switching of tetra- (bromophenyl) porphyrins Performance of oomph-lib in largescale parallel computations 3D instabilities in two-layer flows Structure refinement of nanomaterials Amorphous structures of mirror coatings Edinburgh Soft Matter and Statistical Physics Group DEISA UK Applied Aerodynamics Consortium 2 Hydrogenation Reactions at Metal Surfaces Simulating the control of calcite crystallisation | Novel Asynchronous AlgorithmsEPSRCMulti-layered Abstractions for PDEsEPSRCSustainable Software Generation ToolsEPSRCProperties and Dynamics of Atomic Bose- Einstein CondensatesEPSRCMulti-scale simulation of intense laser plasma interactionsEPSRCLarge Eddy Simulation of LNG Pool FiresEPSRCLES of supersonic jetsEPSRCConformational switching of tetra- (bromophenyl) porphyrinsEPSRCPerformance of oomph-lib in largescale parallel computationsEPSRC3D instabilities in two-layer flowsEPSRCStructure refinement of nanomaterialsEPSRCAmorphous structures of mirror coatingsEPSRCEdinburgh Soft Matter and Statistical Physics GroupEPSRCUK Applied Aerodynamics Consortium 2EPSRCSimulating the control of calcite crystallisationEPSRC | Novel Asynchronous AlgorithmsEPSRCClass1aMulti-layered Abstractions for PDEsEPSRCClass1aSustainable Software Generation ToolsEPSRCClass1aProperties and Dynamics of Atomic Bose- Einstein CondensatesEPSRCClass1aMulti-scale simulation of intense laser plasma interactionsEPSRCClass1aLarge Eddy Simulation of LNG Pool FiresEPSRCClass1bConformational switching of tetra- (bromophenyl) porphyrinsEPSRCClass1bPerformance of oomph-lib in largescale parallel computationsEPSRCClass2aStructure refinement of nanomaterialsEPSRCClass2aAmorphous structures of mirror coatingsEPSRCClass1aDEISAEPSRCClass1aUK Applied Aerodynamics Consortium 2EPSRCClass1aHydrogenation Reactions at Metal SurfacesEPSRCClass1aSimulating the control of calcite crystallisationEPSRCClass1a | Novel Asynchronous AlgorithmsEPSRCClass1aProf Nicholas J HighamMulti-layered Abstractions for PDEsEPSRCClass1aProf Paul KellySustainable Software Generation ToolsEPSRCClass1aProf Paul KellyProperties and Dynamics of Atomic Bose- Einstein CondensatesEPSRCClass1aDr A WhiteMulti-scale simulation of intense laser plasma interactionsEPSRCClass1aDr Tony ArberLarge Eddy Simulation of LNG Pool FiresEPSRCClass1bProf William DawesConformational switching of tetra- (bromophenyl) porphyrinsEPSRCClass1bProf Mats PerssonPerformance of oomph-lib in largescale parallel computationsEPSRCClass2aDr Tony Arber3D instabilities in two-layer flowsEPSRCClass2aDr Frashant ValluriStructure refinement of nanomaterialsEPSRCClass2aDr for Matts PersonAmorphous structures of mirror coatingsEPSRCClass1aProf Michael CatesDEISAEPSRCClass1aProf Michael CatesDr Siaka DembeleUK Applied Aerodynamics Consortium 2EPSRCClass1aProf Michael CatesUK Applied Aerodynamics consortium 2EPSRCClass1aProf Michael CatesSimulating the control of calcite crystallisationProf.Class1aProf. Angelos | Novel Asynchronous AlgorithmsEPSRCClass1aProf Nicholas J Higham500,000Multi-layered Abstractions for PDEsEPSRCClass1aProf Paul Kelly3,816,000Sustainable Software Generation ToolsEPSRCClass1aProf Paul Kelly20,208,060Properties and Dynamics of Atomic Bose- Einstein CondensatesEPSRCClass1aDr A White69,895,466Multi-scale simulation of intense laser plasma interactionsEPSRCClass1aDr Tony Arber4,872,000Large Eddy Simulation of LNG Pool FiresEPSRCClass1bProf William Dawes2,696,000Conformational switching of tetra- (bromophenyl) porphyrinsEPSRCClass1aProf Matts Persson1,704,960Performance of oomph-lib in largescale parallel computationsEPSRCClass2aProf Matthias Heil300,0003D instabilities in two-layer flowsEPSRCClass2aDr Prashant Valluri701,899Structure refinement of nanomaterialsEPSRCClass1aProf. Peter G Bruce300,000Amorphous structures of mirror coatingsEPSRCClass1aProf Michael Cates4,663DEISAEPSRCClass1aProf Michael Cates4,663DEISAEPSRCClass1aProf. Angelos30,925,323Hydrogenation Reactions at Metal SurfacesEPSRCClass1aProf. AngelosSimulating the control of calcite crystallisationEPSRCClass1aProf. John Harding130,403,522 | Novel Asynchronous AlgorithmsEPSRCClass1aProf Nicholas J Higham500,0000Multi-layered Abstractions for PDEsEPSRCClass1aProf Paul Kelly3,816,0000Sustainable Software Generation ToolsEPSRCClass1aProf Paul Kelly20,208,0600Properties and Dynamics of Atomic Bose- Einstein CondensatesEPSRCClass1aDr A White69,895,4660Multi-scale simulation of intense laser plasma interactionsEPSRCClass1aDr A White69,895,4660Large Eddy Simulation of LNG Pool FiresEPSRCClass1aDr Tony Arber4,872,0000Large Eddy Simulation of LNG Pool FiresEPSRCClass1bProf William Dawes2,696,000155,781Conformational switching of tetra- (bromophenyl) porphyrinsEPSRCClass2aProf Matts Persson1,704,9601,734,321Performance of comph-lib in largescale parallel computationsEPSRCClass2aProf Matthias Heil300,00044,1393D instabilities in two-layer flowsEPSRCClass2aProf Prest G Bruce300,0000Amorphous structures of mirror coatingsEPSRCClass1aProf Michael Cates4,6636,171DEISAEPSRCClass1aDr Nick Hills30,925,32320,468,761Hydrogenation Reactions at Metal SurfacesEPSRCClass1aProf Angelos Michael Cates50,000,00041,243,007Simulating the control of calcite crystallisationEPSRCClass1aProf Angelos Micha |

| Code | Title | Funding Body | Class | PI | Total AUs allocated | AUs used | AUs left |
|---------|--|-----------------|--------------|-------------------------------|---------------------|-------------|-------------|
| e77 | Porting of DFT/GW Codes | EPSRC | Class2a | Prof Maria Merlyne DeSouza | 209,662 | 60,676 | 148,986 |
| e82 | ONETEP: linear-scaling method on High Performance Computers | EPSRC | Class1b | Dr Peter Haynes | 1,105,352 | 396,427 | 708,925 |
| e84 | Vortical Mode Interactions | EPSRC | Class1a | Dr Tamer Zaki | 9,600,000 | 503,811 | 9,096,189 |
| e85 | Study of Interacting Turbulent Flames | EPSRC | Class1a | Dr N Swaminathan | 8,088,610 | 2,122,695 | 5,965,915 |
| e89 | Support for UK Car-Parrinello Consortium | EPSRC | Class1a | Dr Matt Probert | 360,000,001 | 149,818,264 | 210,181,737 |
| e92 | Dynamo Action In Compressible Convection | EPSRC | Class1a | Mr Paul Bushby | 4,075,000 | 896,690 | 3,178,310 |
| y08 | Testing | EPSRC | Early use | Dr David Jenkins | 1,000 | 0 | 1,000 |
| NERC | Projects | | | | | | |
| n04 | Shelf Seas Consortium | NERC | Class1a | Dr Roger Proctor | 88,202,935 | 59,566,591 | 28,636,344 |
| n01 | Global Ocean Modelling Consortium | NERC | Class1a | Dr Thomas Anderson | 89,243,840 | 49,172,203 | 40,071,637 |
| n02 | NCAS (National Centre for Atmospheric Science) | NERC | Class1a | Dr Lois Steenman- Clark | 258,768,327 | 190,628,387 | 68,139,940 |
| n03 | Computational Mineral Physics Consortium | NERC | Class1a | Prof John P Brodholt | 284,142,416 | 206,515,914 | 77,626,502 |
| u01 | Melting of MgSiO3 Perovskite | NERC | Early use | Prof John P Brodholt | 11,000,000 | 11,018,423 | -18,423 |
| BBSRC | Projects | | | | | | |
| b08 | Int BioSim | BBSRC | Class1a | Mr Mark M Sansom | 866,000 | 909,998 | -43,998 |
| b100 | Widening the BBSRC HPC User Base | BBSRC | Class1a | Dr Michael Ball | 10,000,000 | 632,465 | 9,367,535 |
| Externa | al Projects | | | | | | · |
| x01 | HPC-Europa | External | Class1a | Dr Judy Hardy | 16,415,790 | 6,916,413 | 9,499,377 |
| HECTo | R_3Q10 | 1 | 1 | Page 21 of 22 | 1 | |] |

| Code | Title | Funding Body | Class | PI | Total AUs allocated | AUs used | AUs left |
|---------|---|-----------------|---------|--------------------|---------------------|-----------|-----------|
| e168 | TEXT | External | Service | Dr Mark Bull | 1,500,000 | 0 | 1,500,000 |
| x05 | FIOS | External | Class1a | Mr Davy Virdee | 1,130,100 | 1,074,930 | 55,170 |
| t01 | NIMES: New Improved Muds from Environmental Sources. | External | Class1a | Dr Chris Greenwell | 4,113,669 | 4,245,424 | -131,755 |
| Directo | r's Time Projects | | | | | | |
| d03 | EUFORIA | DirectorsTime | Service | Mr Adrian Jackson | 2,200,000 | 1,587,951 | 612,049 |
| d04 | MSc in HPC | DirectorsTime | Service | Dr David Henty | 343,500 | 204,567 | 138,933 |
| d15 | HPC-GAP | DirectorsTime | Service | Dr David Henty | 2,033 | 1,037 | 996 |
| d16 | ETC | DirectorsTime | Service | Dr Lorna Smith | 501,000 | 133,964 | 367,036 |
| d18 | FireGrid HPC | DirectorsTime | Service | Prof Arthur S Trew | 600,001 | 250,303 | 349,698 |
| d19 | OpenFOAM Demo | DirectorsTime | Service | Dr Alan Gray | 950,000 | 396,957 | 553,043 |
| d20 | CSCS | DirectorsTime | Service | Dr Alan Gray | 50,000 | 0 | 50,000 |
| d21 | GADGET | DirectorsTime | Service | Dr Adrian Jenkins | 1,000,001 | 18,584 | 981,417 |
| d23 | TEXT FP7 | DirectorsTime | Service | Dr Mark Bull | 1,500,000 | 9,625 | 1,490,375 |
| d24 | SBSI | DirectorsTime | Service | Dr Stephen Gilmore | 2,000,000 | 106,359 | 1,893,641 |
| y09 | Director's Time | DirectorsTime | Service | Prof Arthur S Trew | 29,685,133 | 82,538 | 764,170 |