

EPSRC UK National Service for Computational Chemistry Software at Imperial College London

Funding period: 1st February 2011 – 31st January 2016

EPSRC Reference: EP/J003921/1

Key Performance Indices (KPI) for the period of 1st February 2012 to 31st January 2013

	Feb-Apr	May-Jul	Aug-Oct	Nov-Jan
A) No. of Separate Uni. Res. Group	54	48	53	50
B) Percentage Uptime of Total Available Time	99.8% (Magellan) 100% (Columbus)	100% (Magellan) 99.3% (Columbus)	100% (Magellan) 99.47% (Columbus)	91.9% (Columbus)^
C) Percentage of Training Requests Responded to within Stated Window	100%	100%	100%	100%
D) Percentage of Training Requests Delivered within Stated Window	100%	100%	100%	100%
E) Percentage of Computer Access Requests Responded to within Stated Window	100%	100%	100%	100%
F) Percentage of Computer Access Requests Accepted	100%	100%	100%	100%
G) Average / Peak Loading	132(59%)/222(99%) (Magellan) 139(27%)/387(76%) (Columbus)	100(45%)/220(98%) (Magellan) 178(35%)/462(90%) (Columbus)	47(21%)/155(69%) (Magellan) 191(37%)/483(95%) (Columbus)	163(32%)/530(104%) (Columbus)^^
H) Number of Customer Complaints / Approvals*	0/0	0/0	0/0	0/0
I) Number of Publications**	24	10	7	7

*No complaints/approvals received from users. An annual user survey has been sent to users (See 4_NSCCS Annual User Satisfaction Survey 2013.pdf for details.) **Publications reported during the period (See 2_Publications_Reported_Year2.pdf for a full list). ^Columbus was not available during the operating system upgrade in January 2013, hence the reduced uptime. ^^More processes eligible to run than available CPUs. If there are more threads than CPUs some threads will have to wait for a slice of a CPU to be allotted before that can do anything and the load average will be greater than the number of CPUs.

The KPIs are:

A) The Number of Individual Researchers and University Research Groups [“Users”] that have been in contact with Imperial College regarding EPSRC UK NSCCS (e.g. for advice, guidance etc) and/or have made use of the EPSRC UK NSCCS Service in that Period. This should be expressed as a Total Number for that period (If it is possible to split the total number into EPSRC UK NSCCS Users and EPSRC UK NSCCS Enquiries then this would be advantageous). The number reported is that of “Users” which have made use of the EPSRC UK NSCCS Service in that Period.

B) The Uptime (or Downtime) of the EPSRC UK NSCCS Equipment within the period.

This will be expressed as a percentage of the Total Available Time within that Period.

C) Percentage of Training Requests Responded to within Stated Window

D) Percentage of Training Requests Delivered within Stated Window

E) Percentage of Computer Access Requests Responded to within Stated Window

F) Percentage of Computer Access Requests Accepted

G) Average / Peak Loading (See Figures 1-4 for details)

H) Number of Customer Complaints / Approvals (See 4_NSCCS Annual User Satisfaction Survey 2013.pdf)

I) Number of Publications (including examples of Key Publications with acknowledgement of EPSRC UK NSCCS Service) (See 2_Publications_Reported_Year2.pdf)

J) Annual Data - Identification & Load of Software usage (See Figure 5 for details)

K) Annual Data - Identification of Spectrum of Users Types & Departmental Affiliation (See Figures 6-8 for details)

G) Average / Peak Loading

The ganglia load graph shown in Figure 1 & 2 gives the load (CPU usage) of the machines for the period of 1st February 2012 to 31st January 2013.

Figures 3 & 4 show the load of the queuing systems for the period of 1st February 2011 to 31st January 2012.

Magellan

There are 224 CPUs with 212 dedicated to batch work. This gives 35,616 hours a week. Working on an overall average for the year of 98% of time being scheduled availability, i.e. approx 8 days a year outage for scheduled developments etc, this gives 34,903 as the weekly available hours. *All batch queues inactivated and no jobs running by the end of 31st October 2012. Magellan was decommissioned at noon on 30th November 2012.*

Columbus

The Altix UV1000 has 512 CPUs with 480 dedicated to batch work. This gives 80,640 hours a week. Working on an overall average for the year of 98% of time being scheduled availability, i.e. approx. 8 days a year outage for scheduled developments, etc., this gives 78,868 as the weekly available hours. Columbus was on trial from 20th February to 10th June 2012 and no CPU charging to active users.

Figure 1. Ganglia load of NSCCS machine (Magellan).

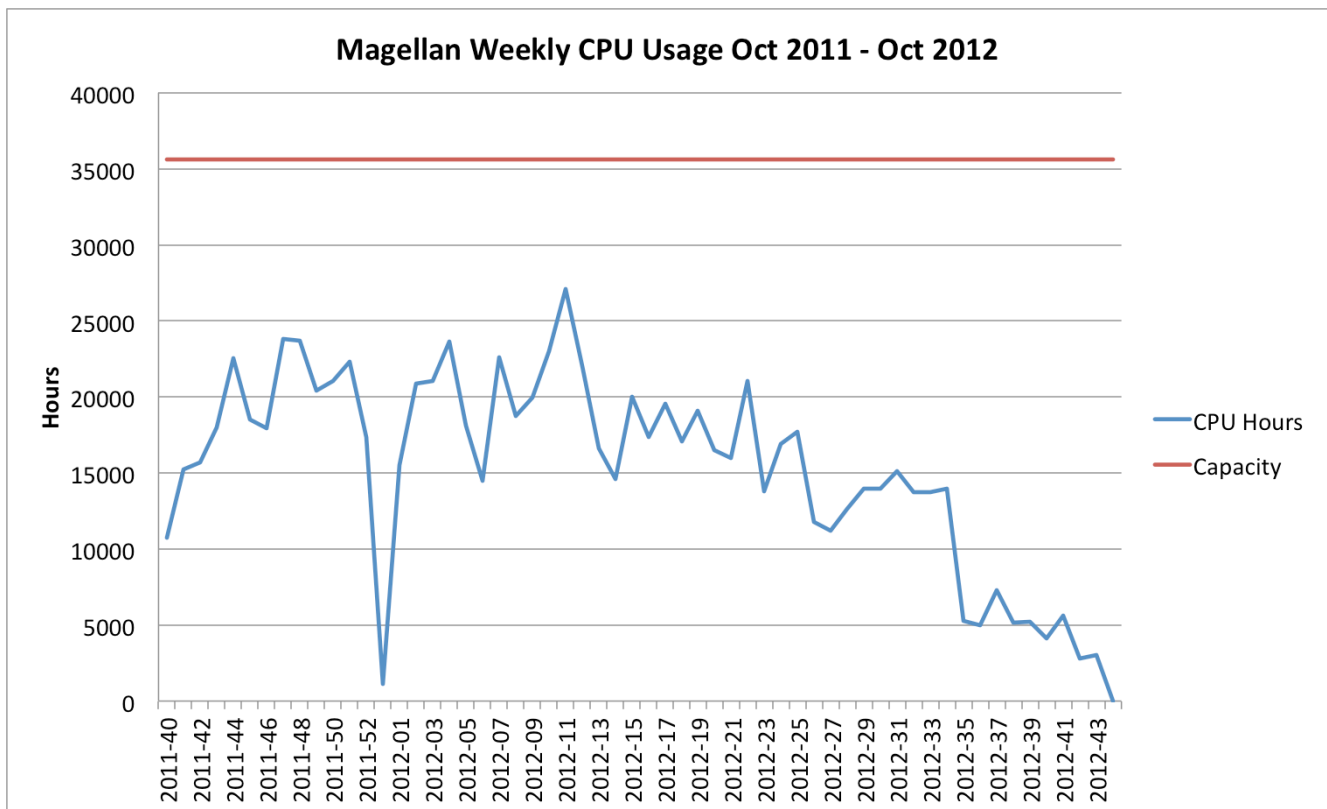


Figure 2. Ganglia load of NSCCS machine (Columbus).

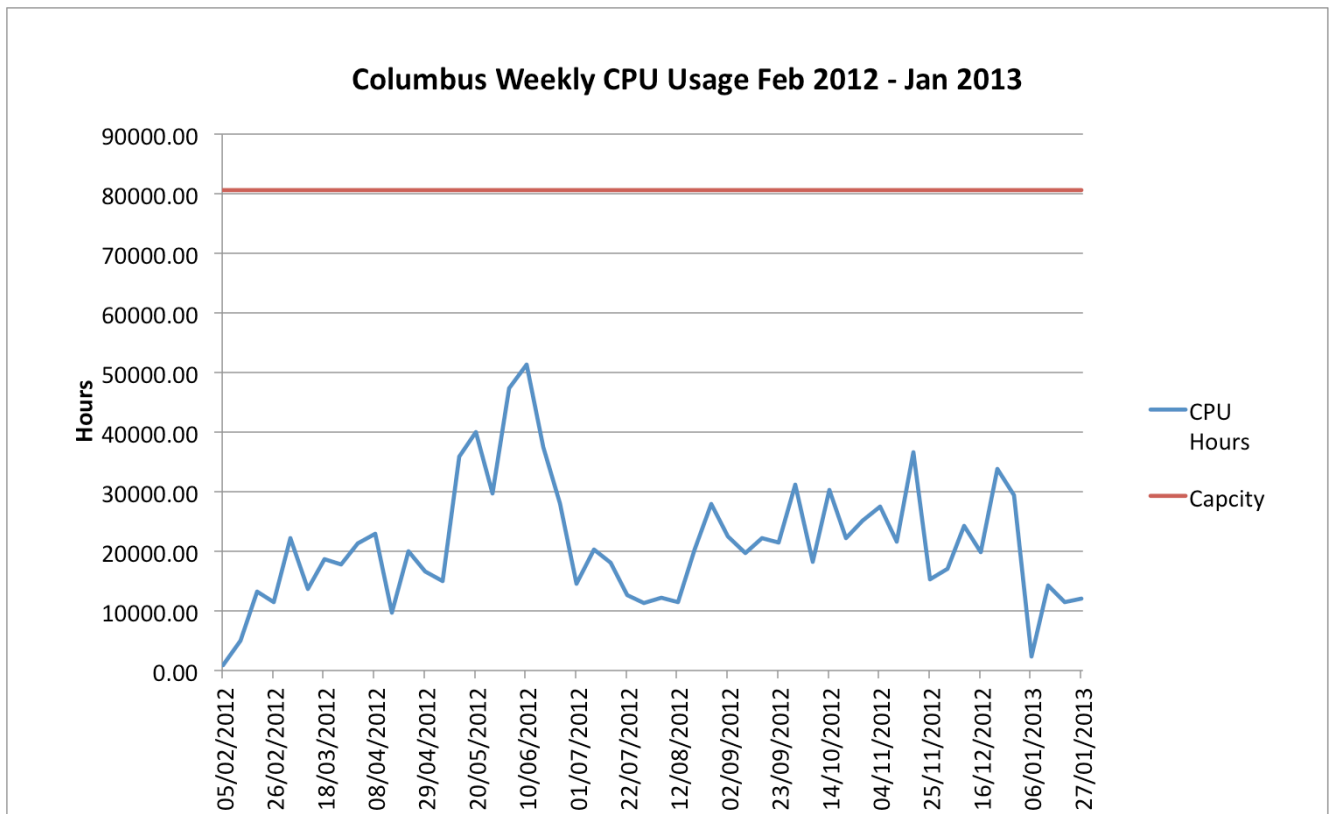


Figure 3. LSF batch load of NSCCS machine (Magellan).

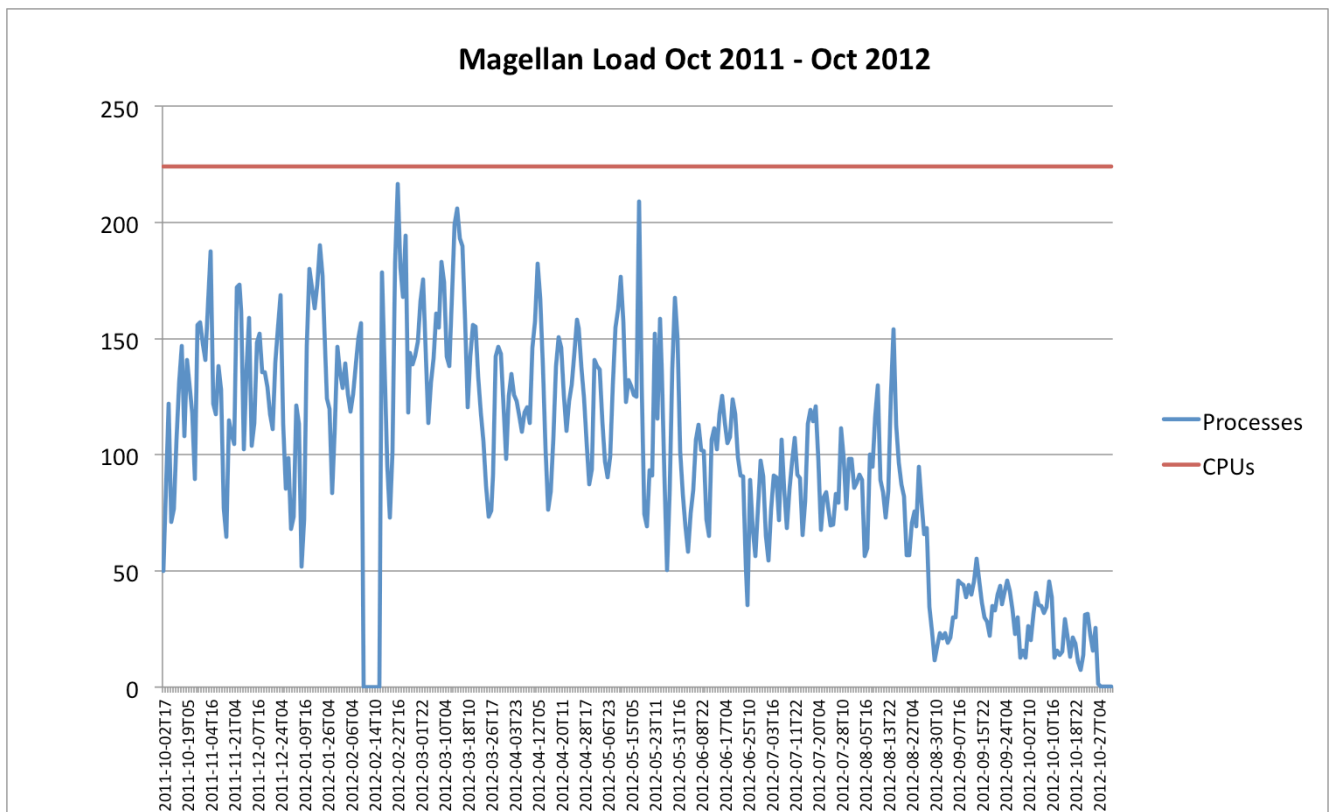
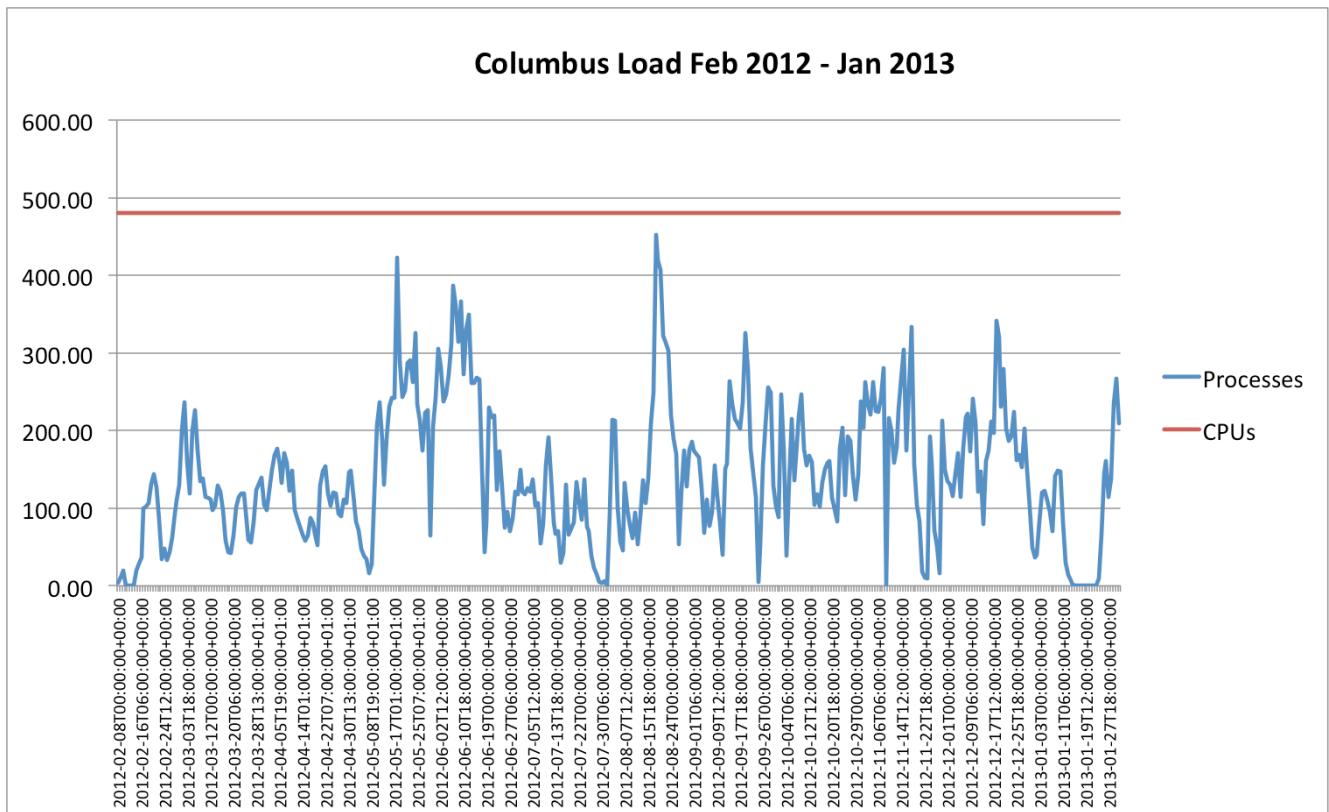


Figure 4. LSF batch load of NSCCS machine (Columbus).

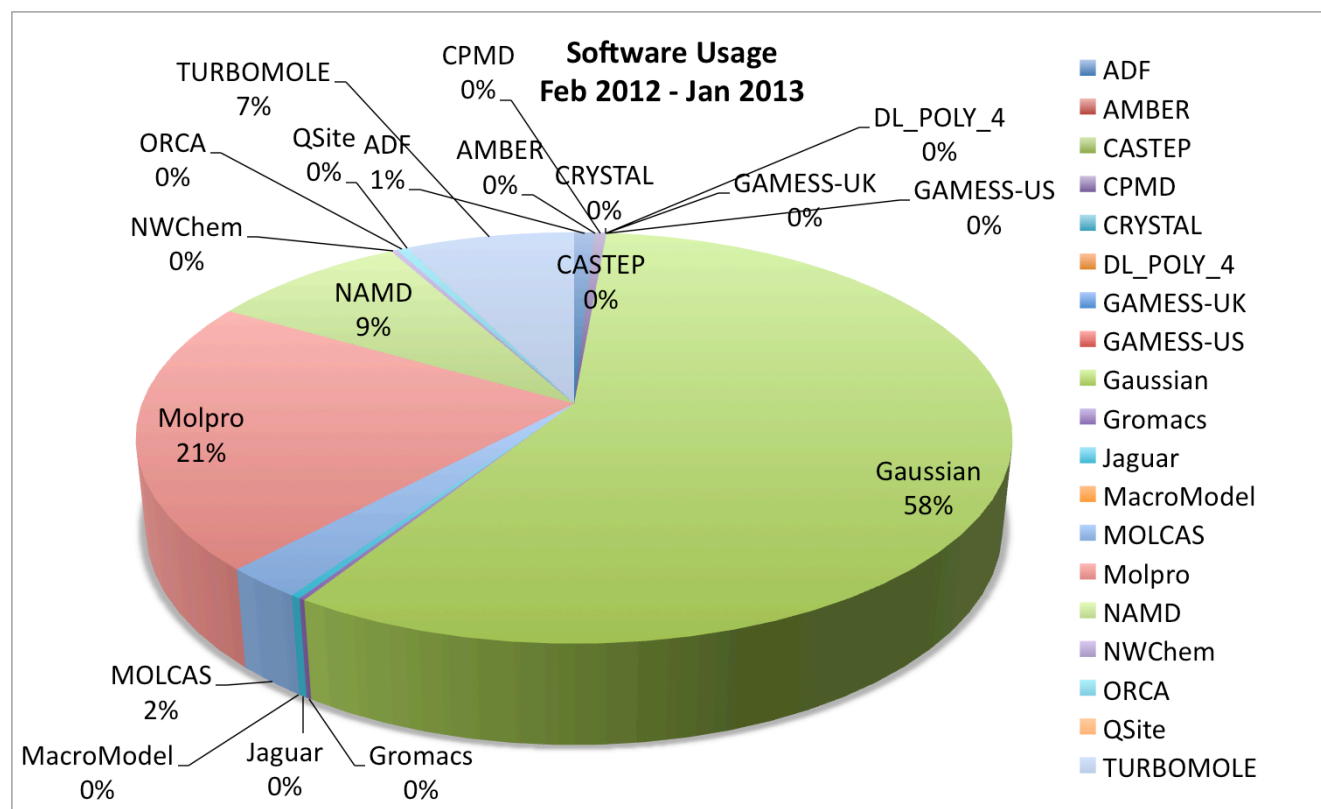


J) Annual Data - Identification & Load of Software usage

The most used software package in terms of computing processing unit (CPU) is Gaussian at 58% as shown in Figure 5.

Figure 5. Software usage for the period of 1st Feb 2011 to 31st January 2012.

*Please note that this is only for illustrative purpose since the logusage script used to gather the data cannot account for all parallel CPU usage. However, the actual CPU usage would have been accounted for by the system. The data presented are combined data from Magellan and Columbus.



Software	Software Usage (%)	Software	Software Usage (%)
ADF	0.9249	Jaguar	0.3213
AMBER	0.0182	MacroModel	0.0025
CASTEP	0.0000	MOLCAS	2.4941
CPMD	0.4236	Molpro	21.3329
CRYSTAL	0.0001	NAMD	8.5772
DL_POLY_4	0.0002	NWChem	0.2716
GAMESS-UK	0.0187	ORCA	0.4861
GAMESS-US	0.0088	QSite	0.0105
Gaussian	57.6144	TURBOMOLE	7.3083
Gromacs	0.1867		

K) Annual Data - Identification of Spectrum of Users Types & Departmental Affiliation

The NSCCS received 61 applications during the second year – 26 pump-priming applications and 33 full applications, 1 was pending and 1 was rejected, from 50 separate research groups from 24 institutions.

Figure 6 gives a break down of research groups per institution. The pie charts in Figures 7 & 8 illustrate the percentages of the different departments and different research categories of the research groups.

Figure 6. Number of research groups per institution.

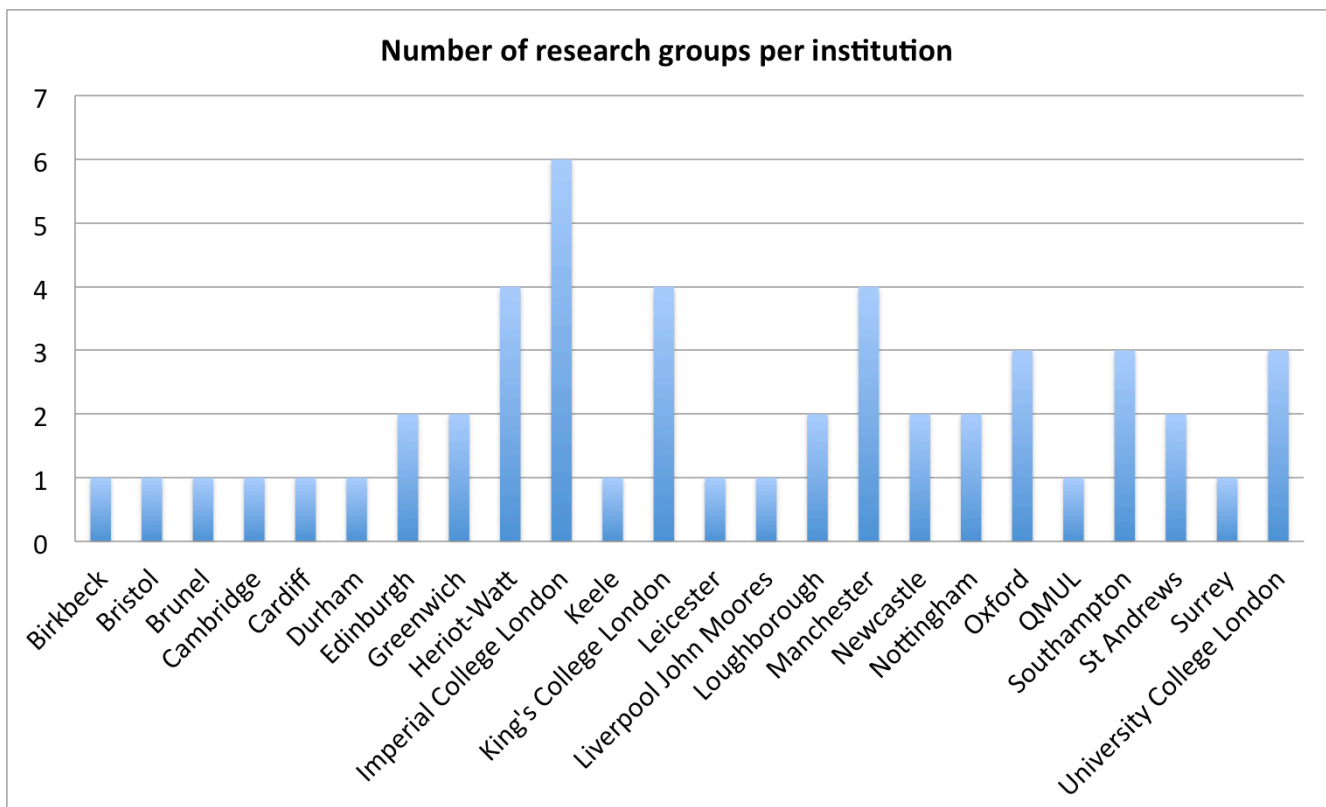


Figure 7. Users' Department listed as a percentage.

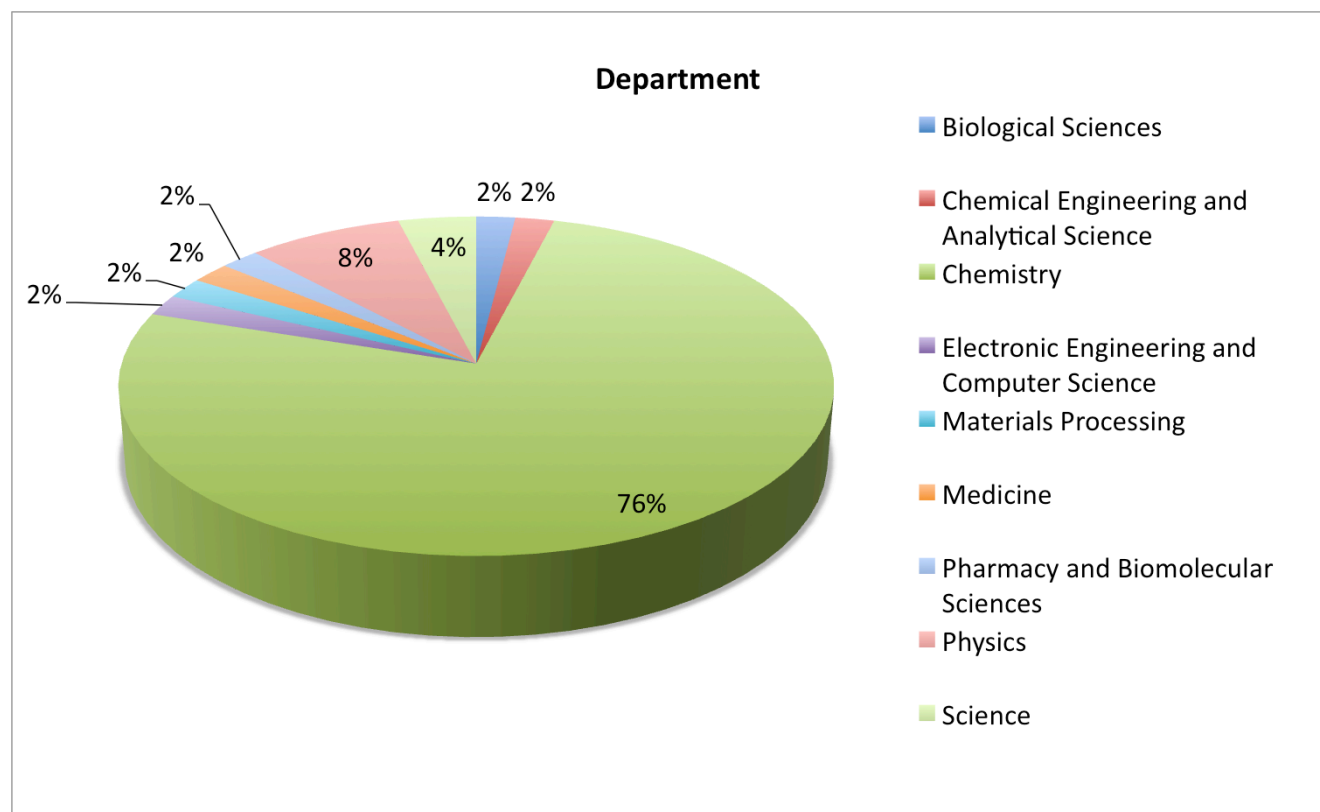


Figure 8. Research categories listed as a percentage.

