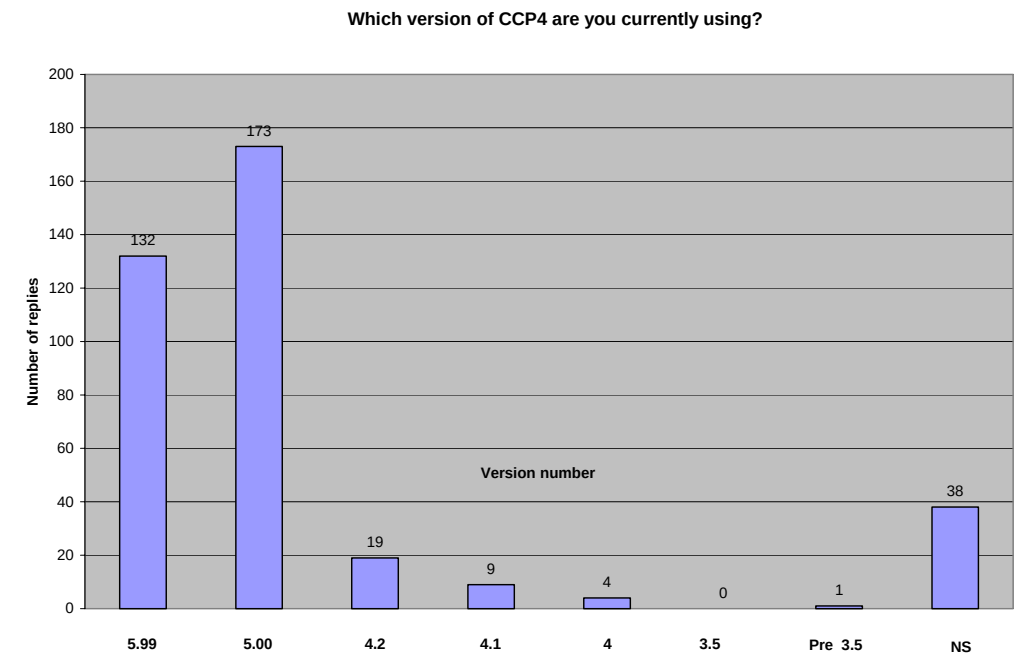
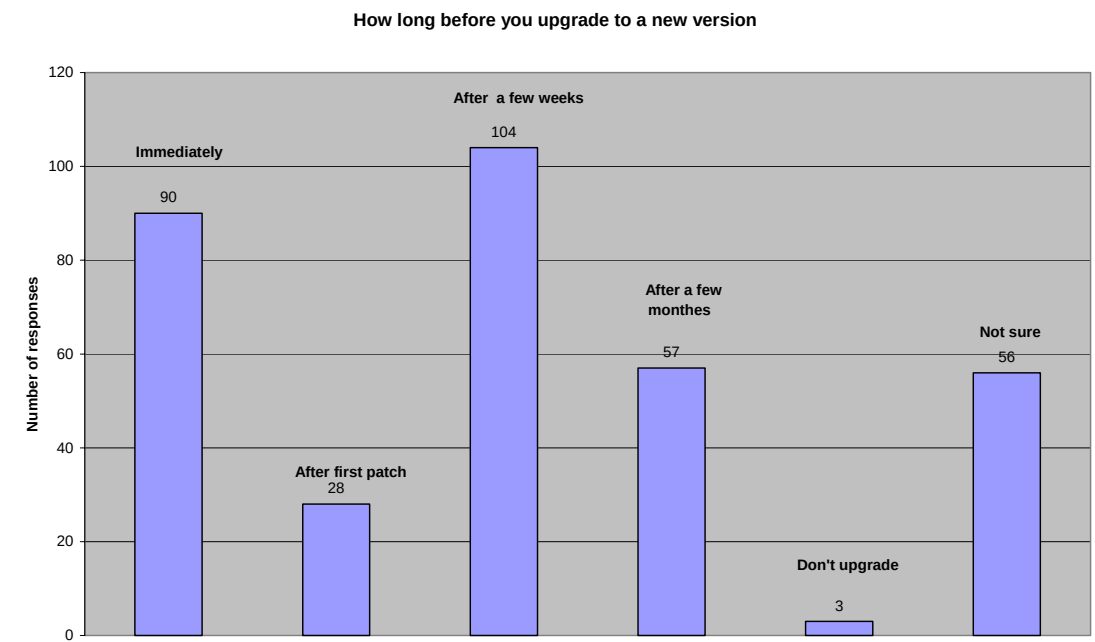


Section A: Installing CCP4

Question 1



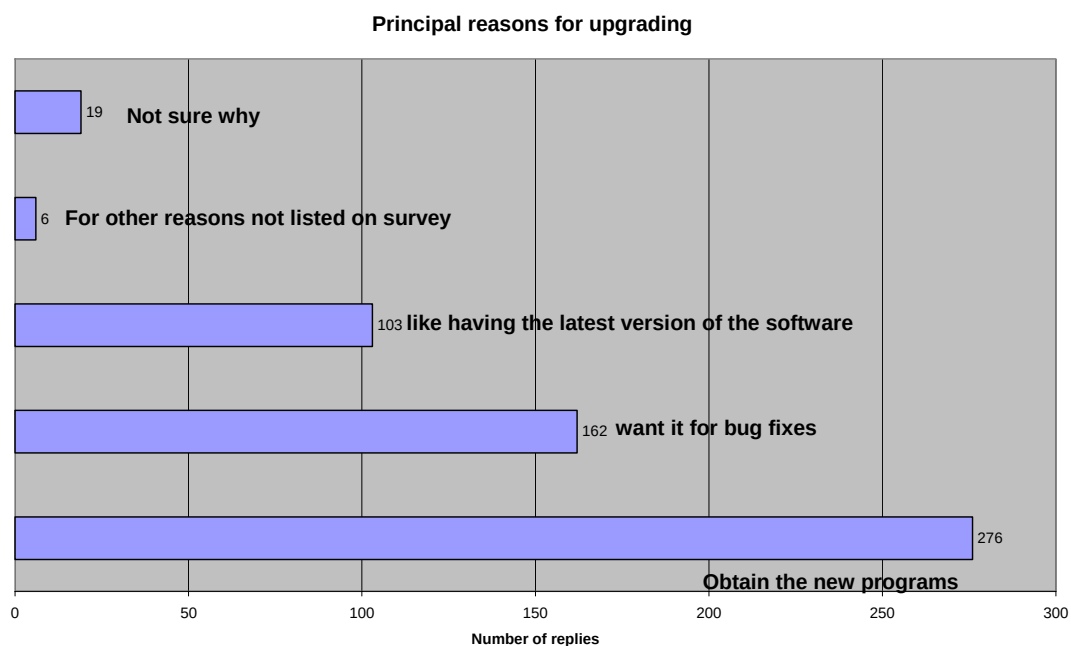
Question 2 :



If you don't upgrade immediately – can you tell us why?

- wait until teething problems with initial installation are worked out
- wait for Fink release
- do not use the package regularly enough to upgrade it immediately
- laziness
- am reliant on a system manager to do the installation
- I wait as long as possible to upgrade as the “old” version works fine for me.
- Issues with the license
- Wait for Windows version to be released.
- If I am not in the middle of a project, then I do upgrade but it depends on my work load.
- It means keeping the “old” version running on an old machine while the new version is being trialled. Not very efficient way to use the new version!
- Different computes get upgraded at different rates.
- We have pipelines and scripts. We don't want to break when working in automated mode.

Question 3: What are your principal reasons for upgrading?



Question 4: Do you ever use developmental or beta versions of the CCP4 software?

33% said yes

69 % said no

Question 5: Do you install CCP4 yourself?

44% said yes

56% said no

Question 5A: If “yes” then which type of installation do you use?

37 % *Build from source code*

63 % *Install using pre-built binaries*

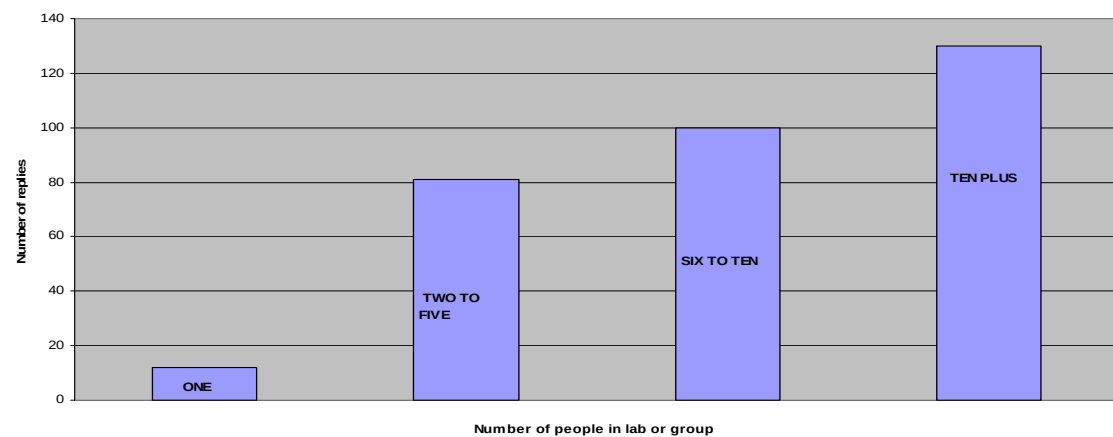
Section B: About your Lab

Question 1: What type of CCP4 license do you have?

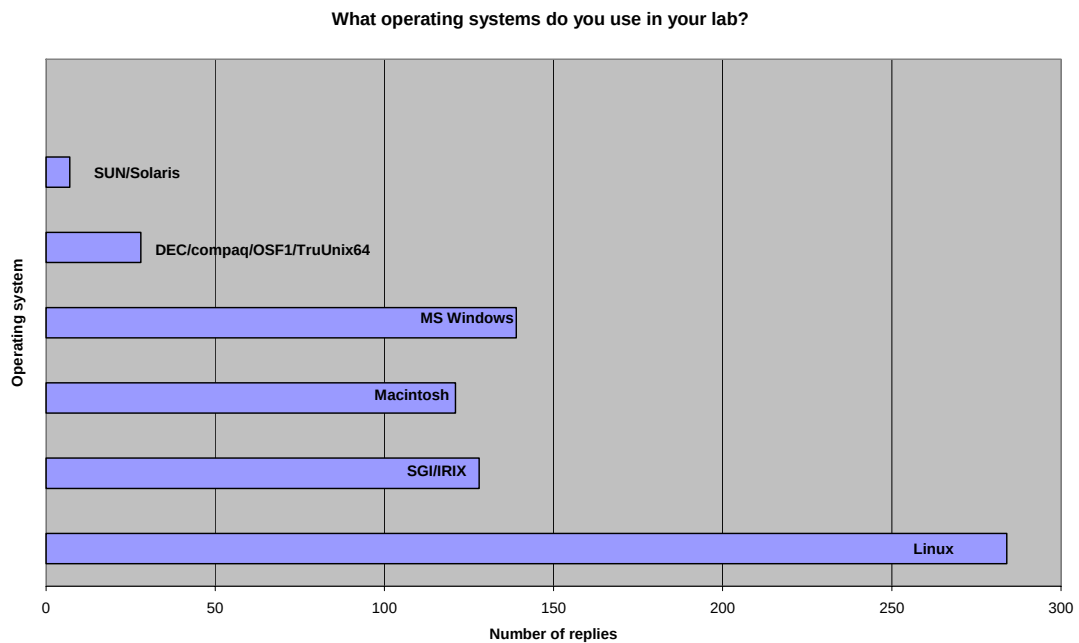
94% have an academic license

6% have a commercial license

Question 2: How many people in your lab or group use CCP4?



Question 3: What type of OS do you use in your lab?



What type of Linux do you use?

REDHAT

SUSE

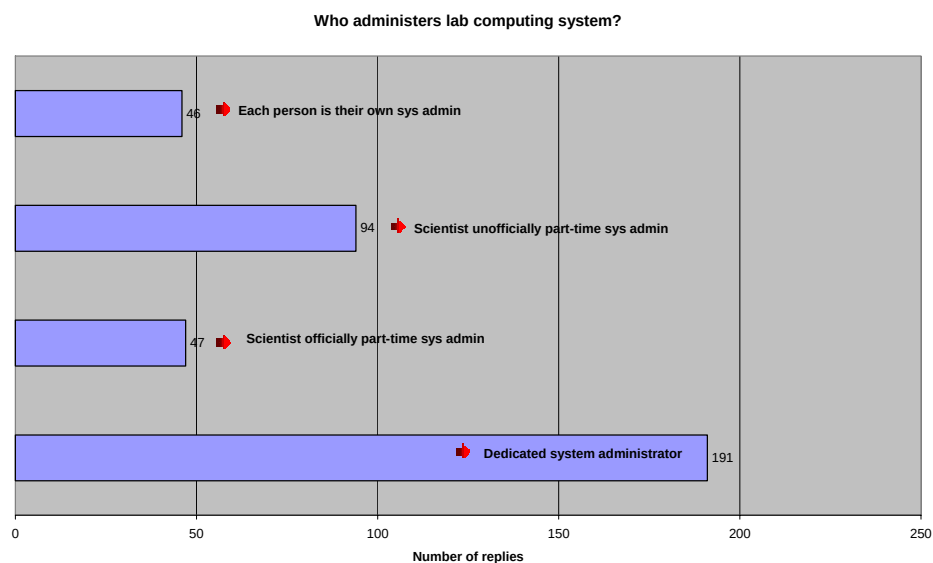
FEDORA

What version of Windows do you operate?

XP

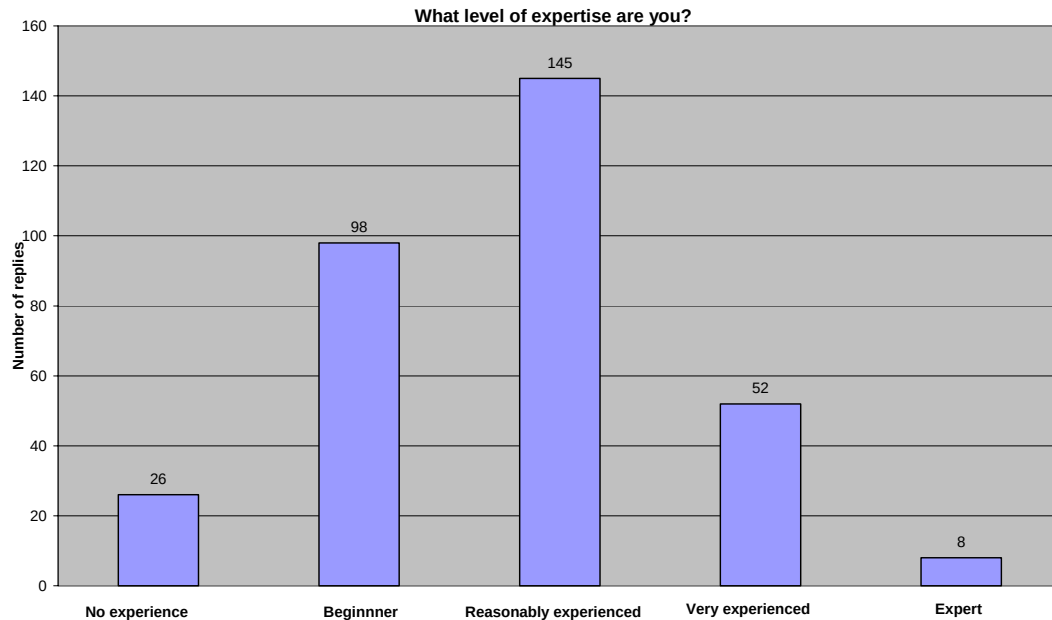
WNT

Question 4: Who administers your lab computing system?



Section C: Using CCP4

Question 1: How would you describe your own level of expertise with using CCP4?



Question 2: Do you use CCP4i as your main way of running CCP4 programs?

78% said yes

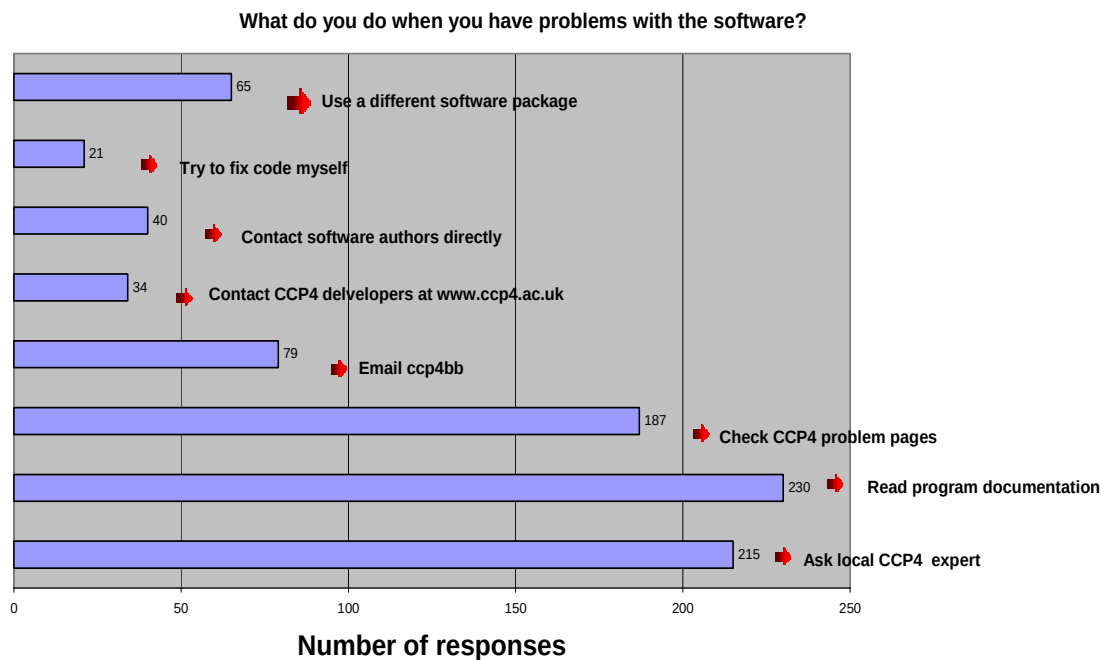
If you answered "no", can you tell us briefly why?

- Still use script for special cases
- No longer running bgms myself
- not experienced enough to feel confident with running it
- Used to be electron crystallographic and MRC software for image proc., better working in script environment.
- like getting hands dirty
- like scripts/automation
- I am a beginner and have not been taught how to use it.
- For some programs eg Refmac csh is easier.
- Scripts are more readily available – process more transparent
- GUI too complicated
- there are a large number of functions not available on the GUI and the (manual) program documentation is set up to use scripts rather than the GUI.

- never got in the habit. Go back and forth to CNS.
- use in house automation software
- still like com files to combine programs
- using custom HTX scripts
- For some of the programs, like Amore we like to use script files.

Question 3: Which are the key programs that you use from CCP4?

Question 4: What do you do when you have problems with the software?



Question 5: What is your favourite feature of the suite?

Availability, completeness, consistent syntax
Simple to use with CCP4, Loggraph gives great way of checking output ie not long tables.
All in one place
Free, well supported, especially with BB.
Inter -compatability
Good that there is a Windows Version available.
Easy programs to use
The Examples
Window based, keeps records of all old jobs.
It's vast store of Programs
Kept up to date
Very User Friendly
Good project management - GUI
Logging/archiving of work
Integration between different programs
Common Formats
State of the Art - Always developing
The simplicity of the web based manual
Self Explanatory
Single Installation for so much stuff
Ethos of CCP4

Flexibility of MTZ Data format is useful
Good mentality of Software
Good for documentation
It's Collaborative
Speed of processing + power of programs.
The Interface and open source
Mosflm, Phaser, CCP4 mg
All features great especially COOT.
New CCP4 mg
Excellent User Friendliness
GUI
Ease of use of CCP4I
Graphical interface CCP4I
Possibility of use between programs
Complete set of Programs that use same file
Indexing of Program output.
Free
Smooth flow of results into next program.
Excellent Quality
Study Weekends

Question 6: What single change or new feature would you like to see?

Better MAD/SAD phasing (new tutorial.)
Better comprehensive documentation.
More needed for first time users (more hints.)
Include all Xstall Programs
Simpler documentation and easy to follow tutorials
MOSFLM in Windows
Better documentation needed for newer programs.
Links to move 'third party' software
Include Mosflm in the GUI
Better File handling system
Integration of CCP4MG and COOT
The Mosflm GUI
Documentation especially for CCP4i, still patchy.
Making Mosflm available for MS Windows.
COOT/MG
Good Automation
CCP4I to be run for diff projects.
Integrating Mosflm
Graphics for building
More example scripts needed.
A Graphical Interface needed.
Resolve like DM
Improve CCP4mg in Windows
CCP4 MG works better

Make sftools easier to follow
Updated Manuals and Protocols
Directories for Projects
Make COOT better
Dummy guide to use software.
Make error messages less cryptic.
A better Manual needed.
Better GUI for Mosflm
More Integration
Better handling of data.
Be able to run data processing packages.
Nicer looking Interface
More informative/simpler files.
Add CNS
Molecular Graphics Improvement
Make it compatible with CNS/PDB Files.
Increase num of options in Graphic Version
Data Collection Software
CCP4MG
Comprehensive Graphics Package
more programs for experimental phasing
More automatic processing for problems.
Automate standard procedures
More updated tutorials.

Question 7: What other non-CCP4 crystallography software do you use most frequently?

The most popular software (and the number of responses) were:

CNS	108
Shelx	68
"O"	51
Pymol	49
XDS	40
HKL 2000	40
Denzo	39
Quanta	26
Solve	49
Mosflm	21
Xtal View	12
ArpWarp	11
Phenix	11

Many other software packages were listed but as they did not have a high enough response (+10) we did not list them.

Question 8: Do you use any of the following CCP4 services and if so, then how useful do you find them?

1. CCP4 Helpdesk ccp4@ccp4.ac.uk
2. CCP4 website www.ccp4.ac.uk
3. CCP4 Bulletin Board CCP4BB
4. CCP4 Problem Pages
5. Newsletters
6. Manual
7. Study Weekend Proceedings