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bragg
institute

ansto in partnership

Australian Nuclear Science & Technology Organisation

Data Analysis Survey 2004



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Survey quote

“...understand the required end-user experience and process before writing a single line of code.”

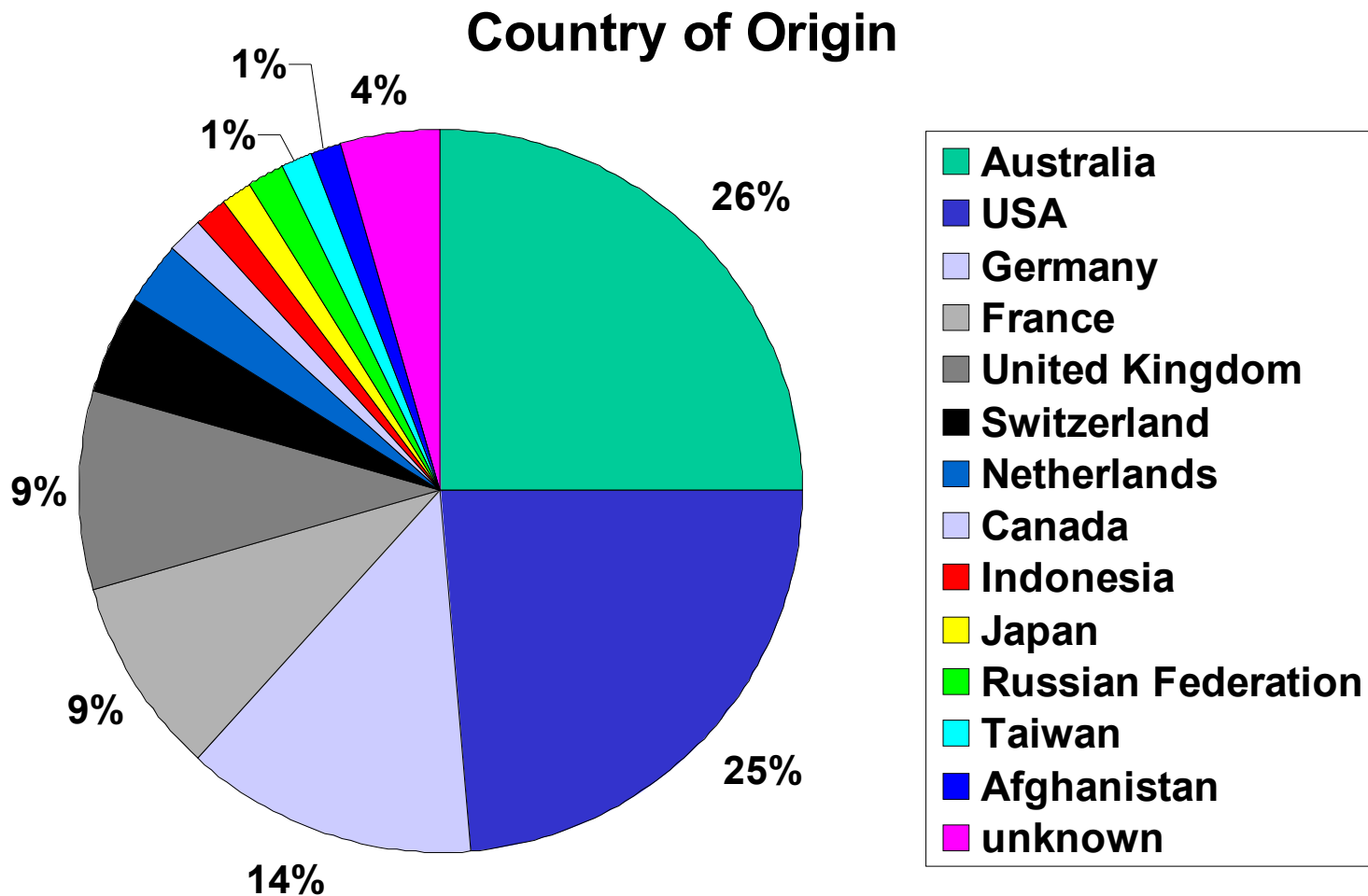
“ GOOD PLANNING AND WIDESPREAD CONSULTATION...”



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Country of origin



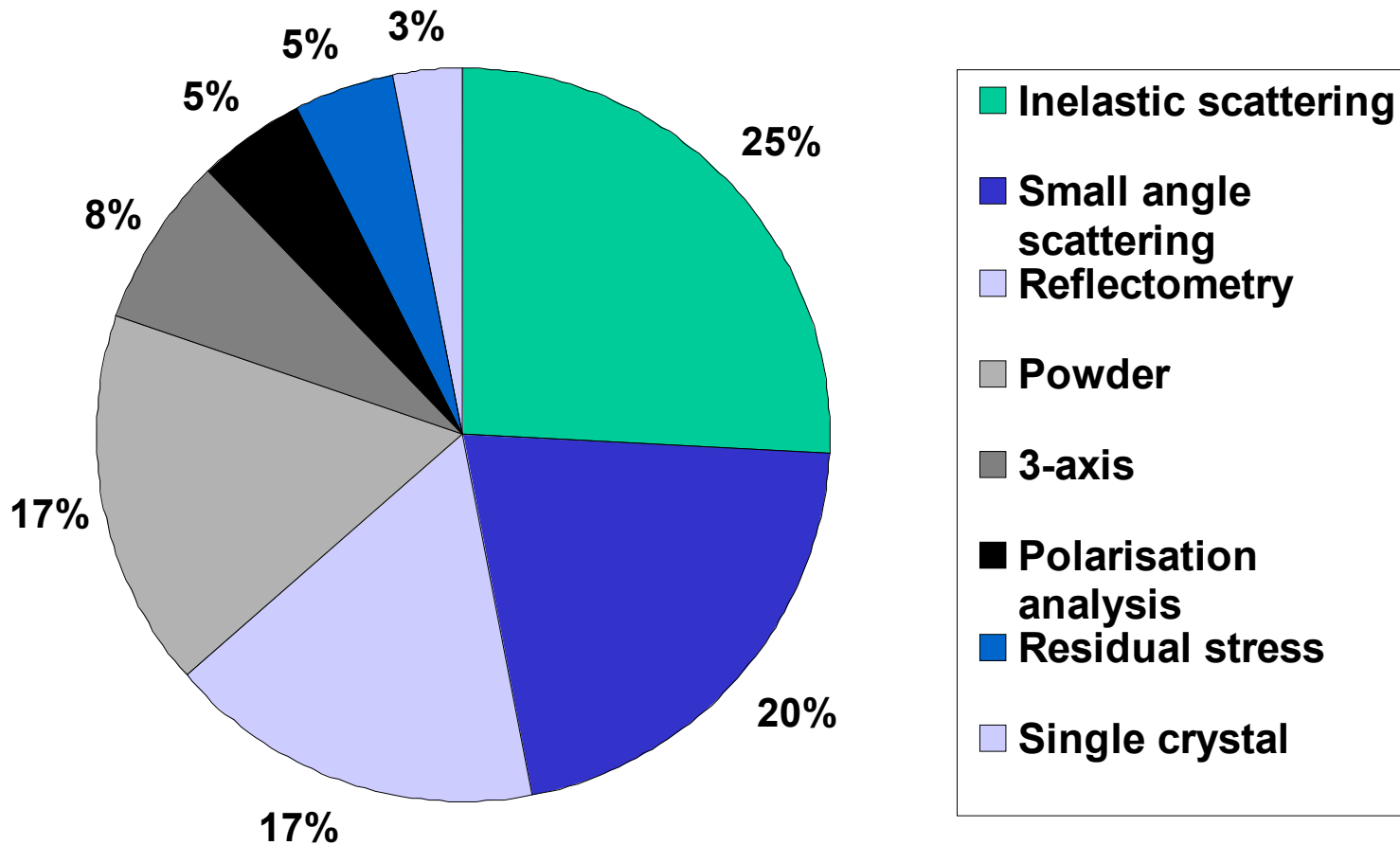


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Technique

Technique



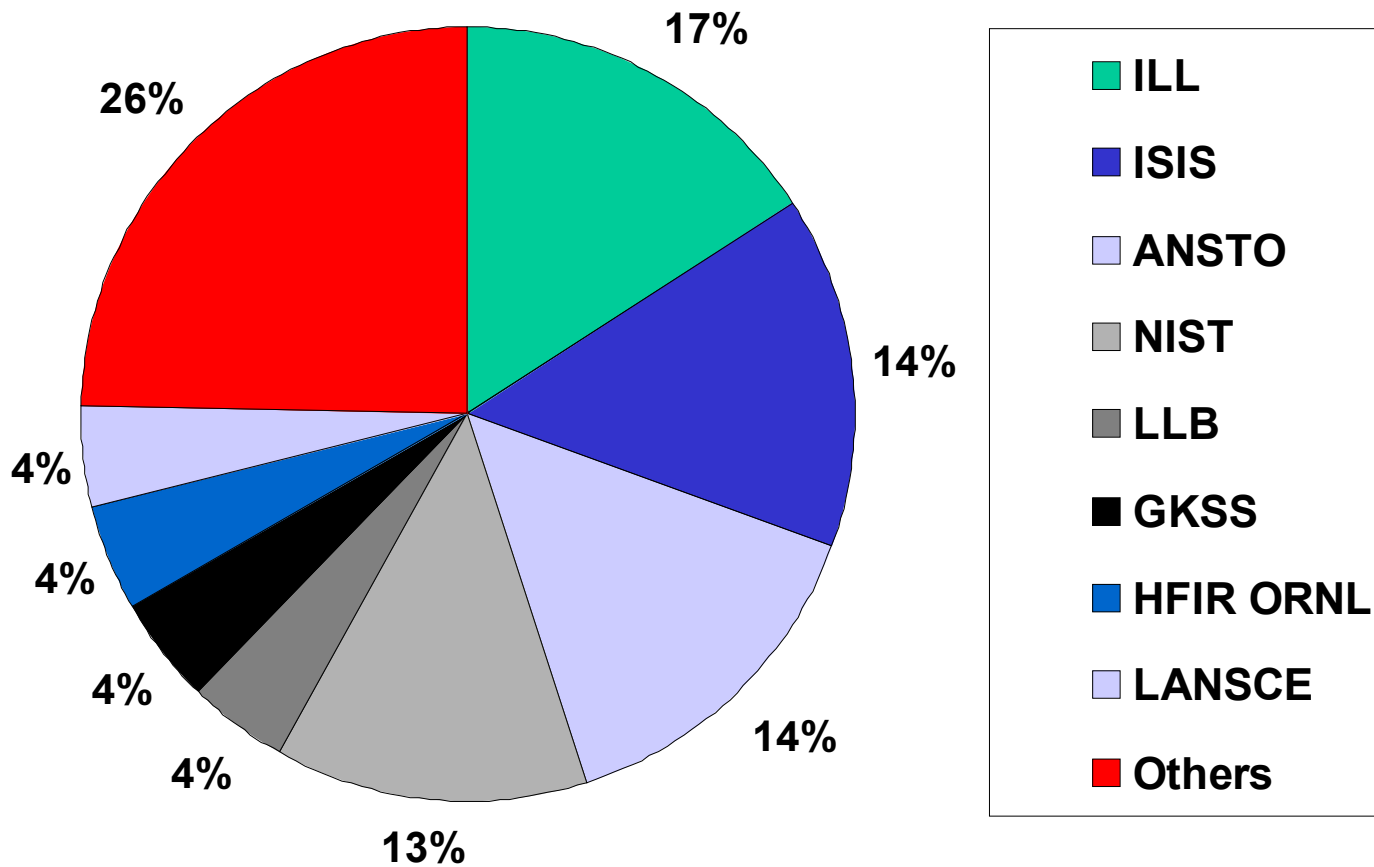


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Primary Institute

Primary Institute



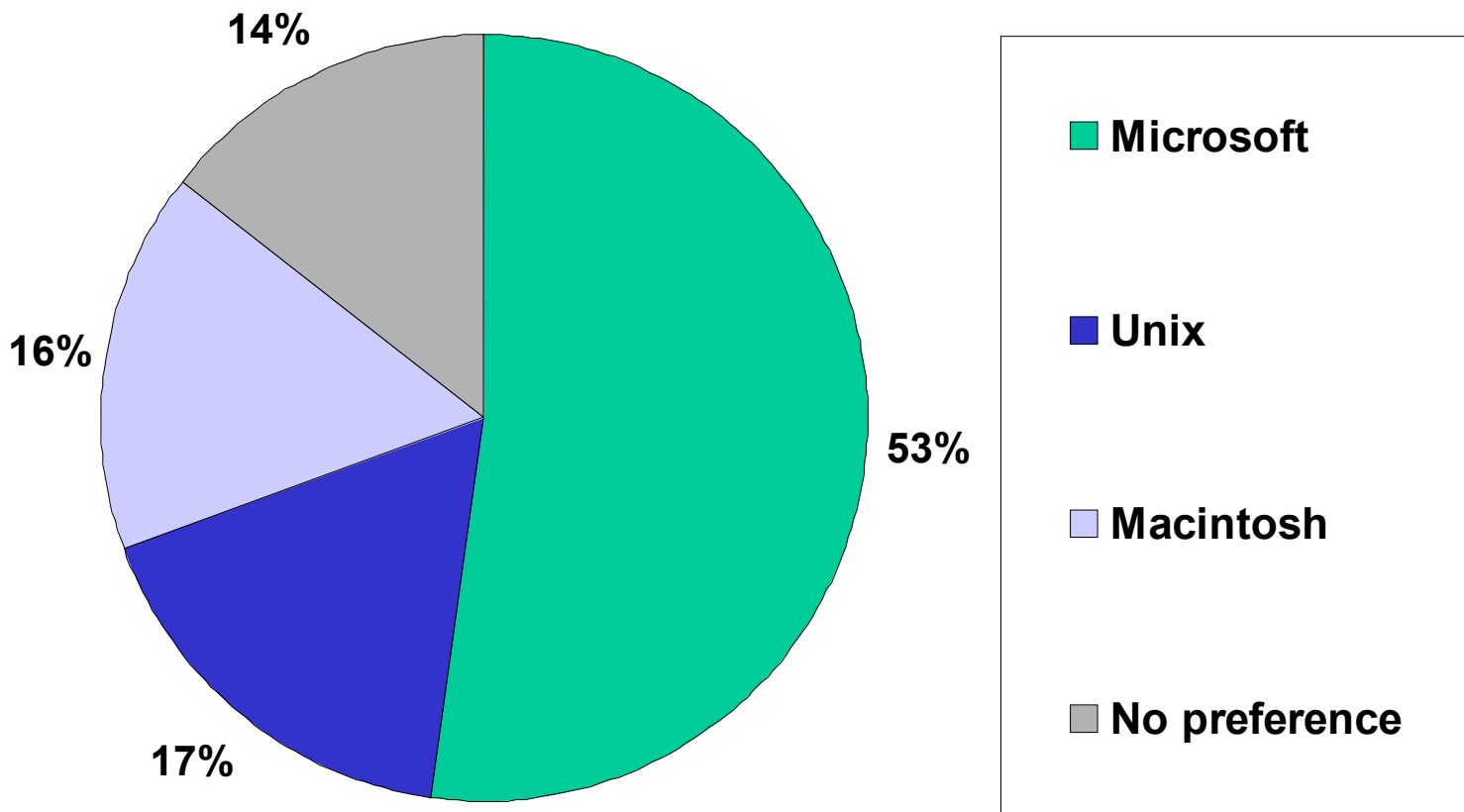


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Preferred operating system

Operating System



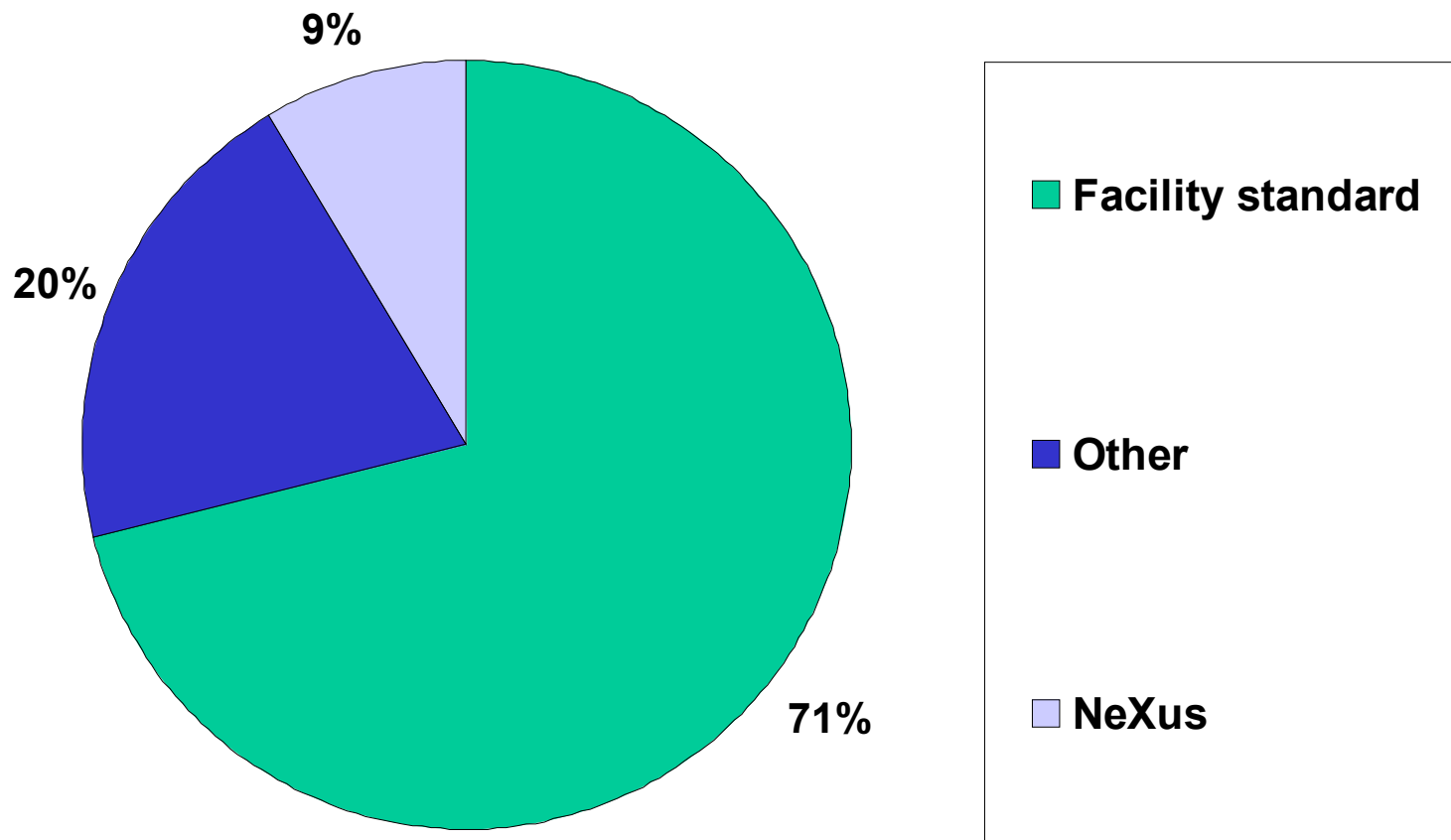


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Data format

Data format





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Platform - visualisation

- 53% use Microsoft Windows
- 54% would use NeXus if available, 19% wouldn't.

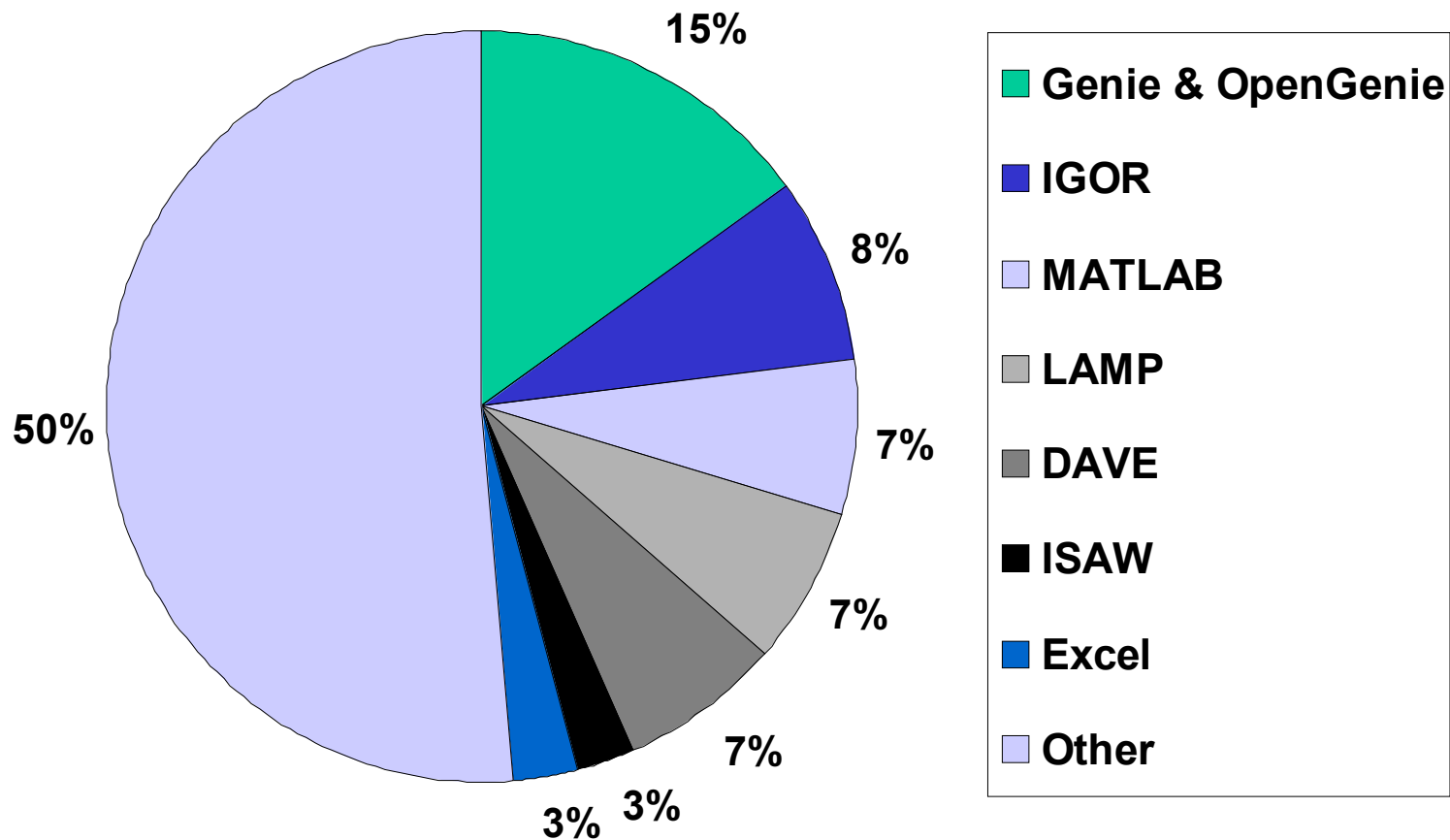


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Best visualisation software

Best visualisation software





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Package popularity

- Nearly half the users would have their requirements fulfilled by supplying 4 packages
- 33% use and prefer OpenGenie and IGOR
- 15% use and prefer LAMP and DAVE



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Package popularity

- 29 packages in “best visualisation” category
- 28 packages in “best analysis” category
- 22 packages overlap best analysis and best visualisation categories
- Total of 47 packages cited by 70 respondents, and doesn't include home grown code and scripts.



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Best data reduction/visualisation

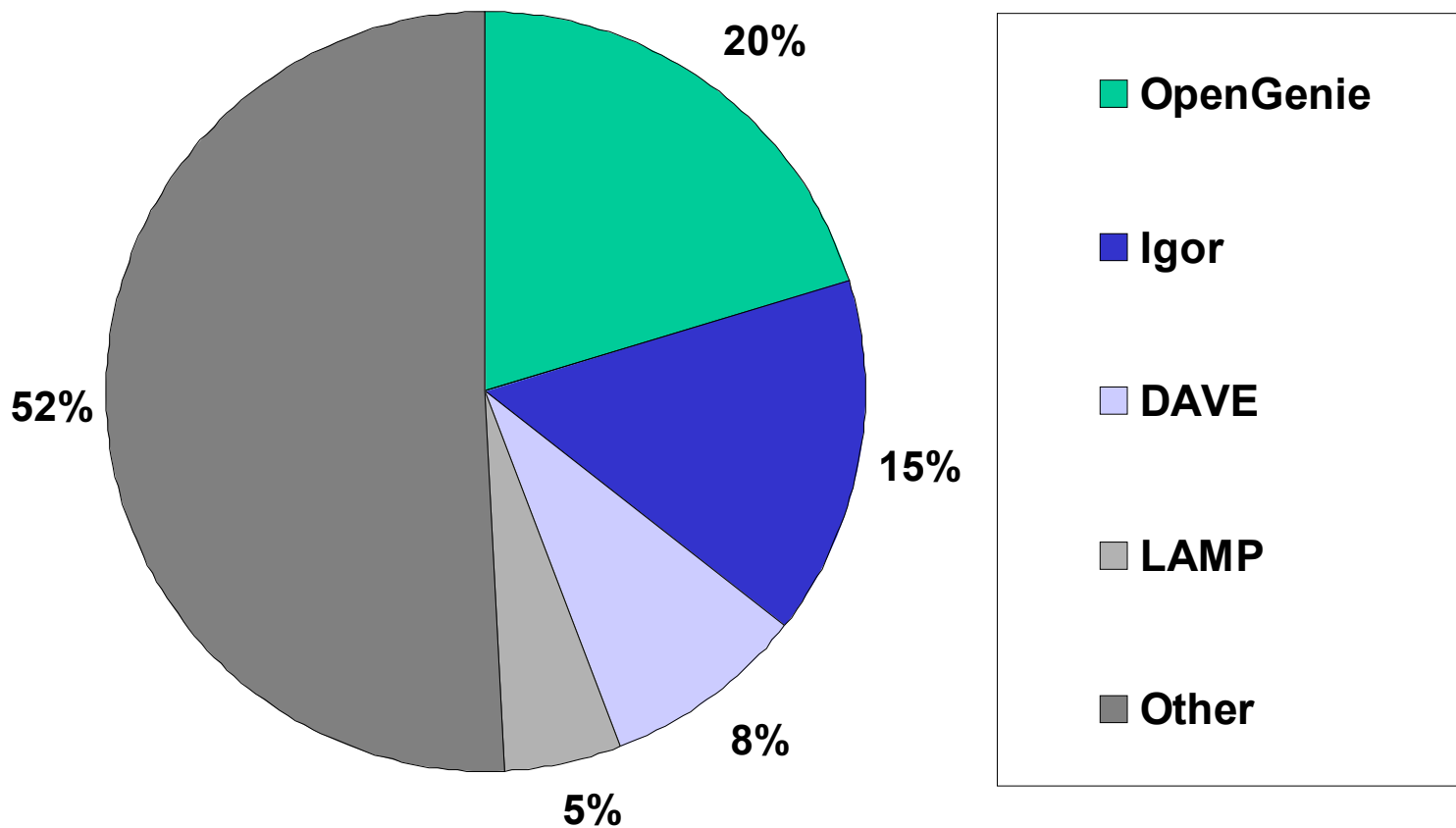
| | | |
|------------------------------|-------------------------------|----------------|
| BEAN | GSAS | Panorama |
| Bruker SAXS | IDL | Peakfit |
| Collette | IGOR | PVWave |
| CrystalMaker | ISAW | PXY |
| DAVE | JADE | Reitica |
| David Cookson's SAXS package | LAMP | Sandra |
| Excel | Mathematica | SHADOW |
| Fullprof | Matlab | SingleCrystal |
| GENIE/Collette | MSLICE/MVIEW/ MFIT | Winplotr |
| gnuplot | Origin | |



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Visualisation package used at facility

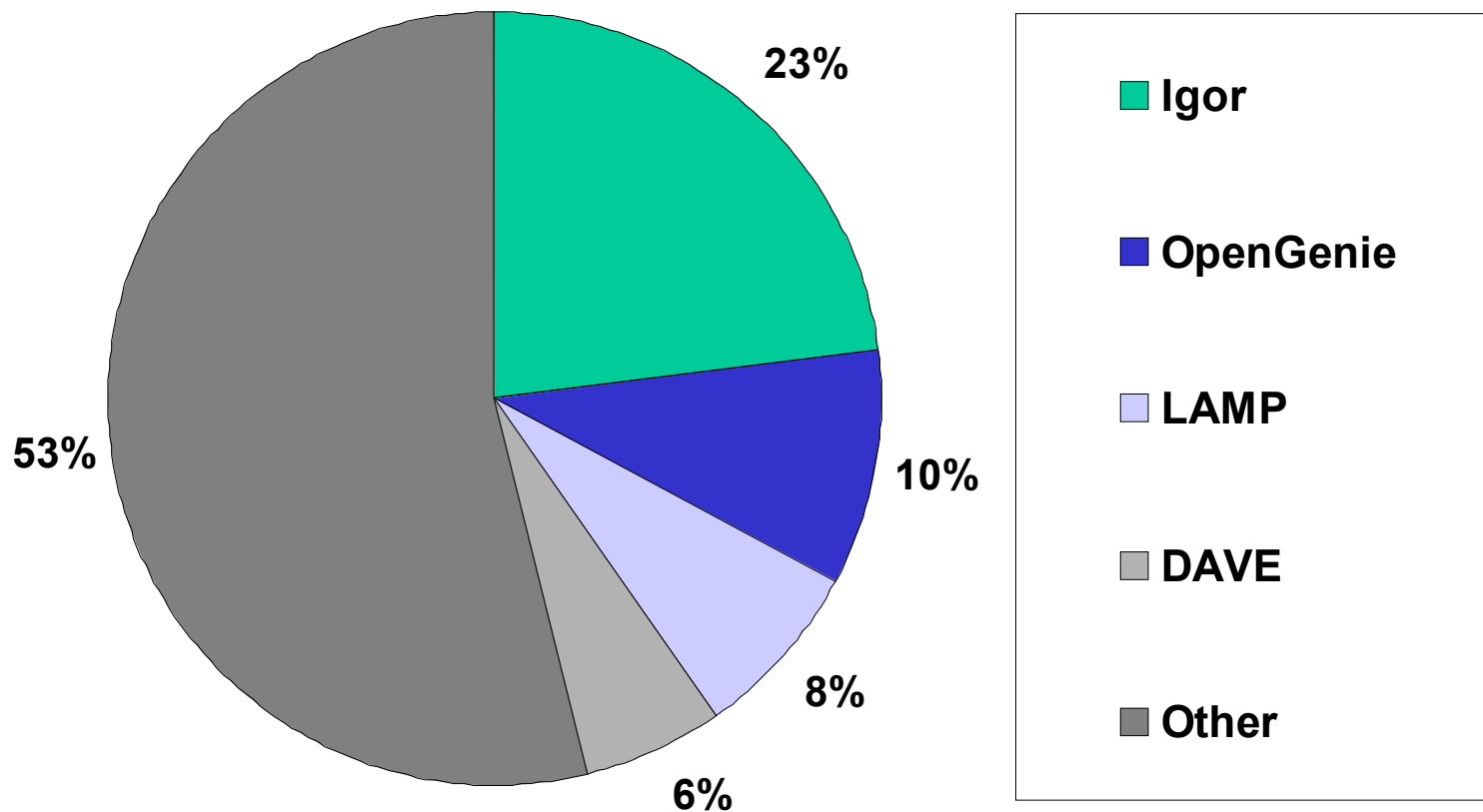




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Visualisation package used at home





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Where and how - visualisation

- 96% do reduction and visualisation at the facility
- 96% do reduction and visualisation at home

- 26% do data visualisation over the internet, but 66% would do it if available

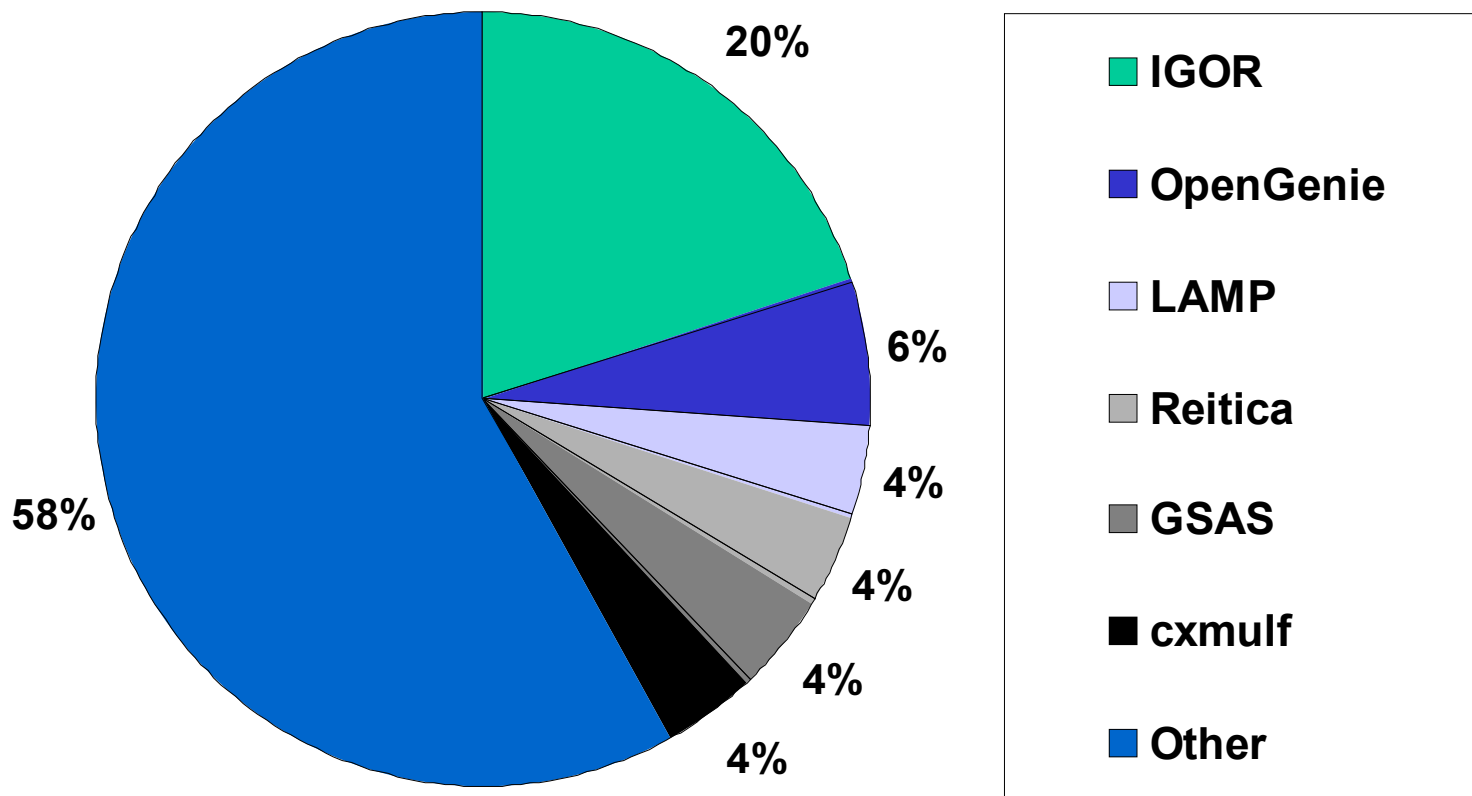


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Best analysis software

Best analysis software





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Best data analysis

| BEAN | GSAS | Origin |
|-----------------|-------------------------------|----------------|
| ccp13 | IDL | Parratt |
| CCSL | IGOR | PXY |
| CXMULF | ISAW | REFSIM |
| D Trek | JADE | Rietica |
| DAVE | LAMP | Sandra |
| Fullprof | LHPM | SHADOW |
| GENIE | Mathematica | SigmaPlot |
| GNOM | Matlab | |
| gnuplot | MSLICE/MVIEW/ MFIT | |



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Platform - analysis

- 62% use Microsoft Windows



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Where and how - analysis

- 85% do analysis at the facility
- 15% say there's not enough time, or use their own programs at home
- 17% do analysis over the internet, but 58% would do it if available

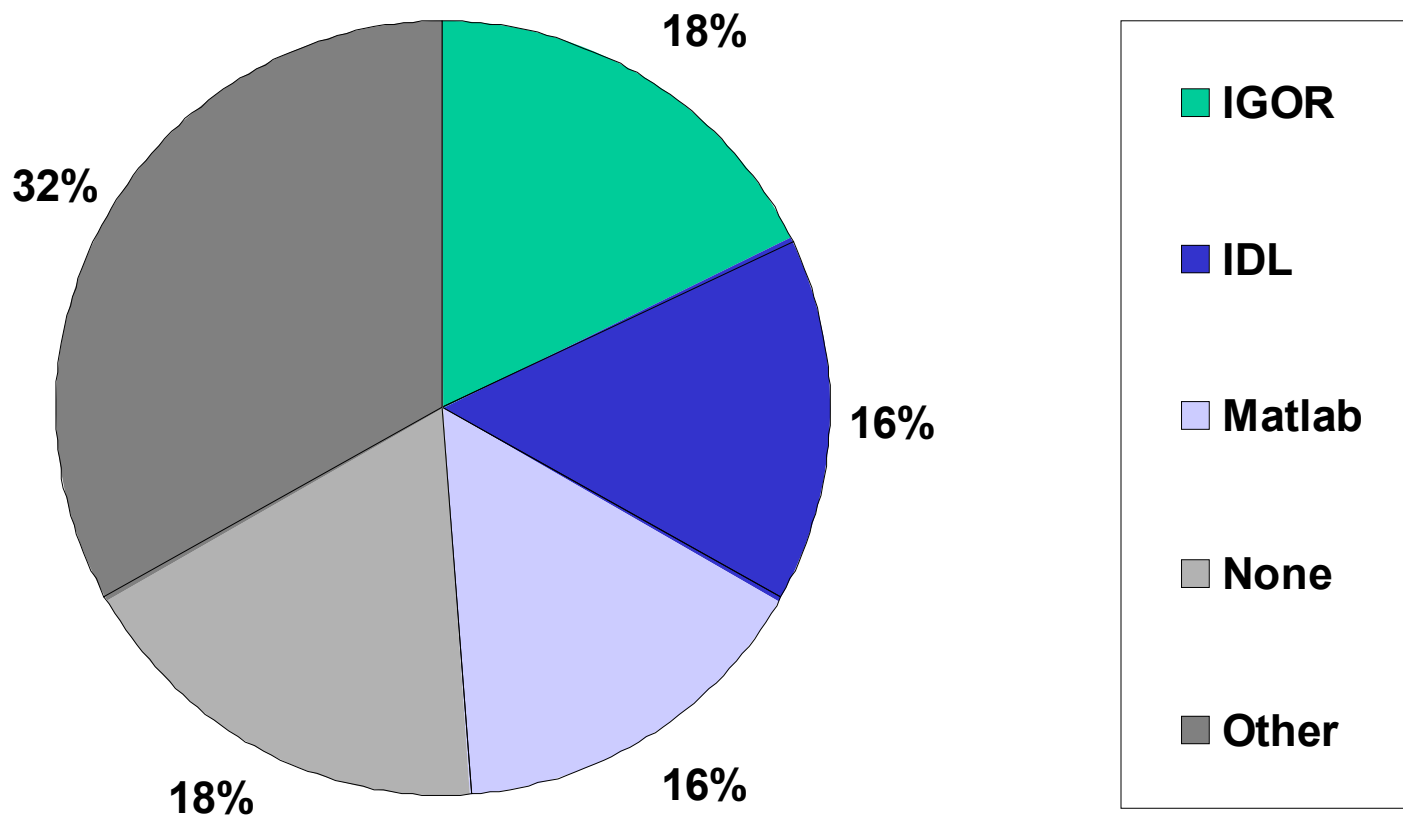


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Data analysis environments

Data analysis environments





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Comments from survey

Categorised into

- Novice/expert users
- Interface
- Graphics
- Standards – data and tools
- Collaboration
- Delivery methods
- Documentation
- Design and architecture
- Pitfalls



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Novice/expert users Cater for both?

“Data visualization, reduction and analysis software should be **easy to use for novice users** and **sophisticated enough** to satisfy the **experienced neutron user..**”

“ease of use (reading in data), functionality..”

“**If it is idiot proof, it is rigid.** If it is flexible needs more know-how. In Igor you can build fixed interface for the first case, but insiders have access to the inner workings. There is only one tool to learn!”

“**Clear instructions** for beginners/occasional users..”

“Access to **expert help.**”

“The users must have a **wider knowledge..**”



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Interface GUI, script or both?

“Prefer Microsoft GUI ... easy to use **GUI**... needs to have a GUI...”

“Analysis software can be made **menu driven** to large extent... combining data visualization and simple data analysis software will be helpful to the users.”

“**Intuitive** (don't have to read a manual/help file), as few mouse clicks as possible, fast, ability to "batch-process“...”

“Make file formats, interfaces and routines as **homogeneous** as possible among **different classes of instruments**...”



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Interface GUI, script or both?

- “**complete packages** so that you do not have to do things between more than one program...”
- “Must be as **customisable** as possible (eg, fitting functions can be user functions) so that analysis can be performed to the scientists requirements..”
- “I believe that it is necessary to have **GUI** tools like MSLICE **layered on top of a well-structured scripting language**. This accommodates both novice users and those doing non-standard analyses. It is preferable if the same scripting (or command-line) environment is available on all instruments...”



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Interface GUI, script or both?

“I don't care much about gui, though I find Windows the least user friendly..”

“**Quit generalised GUI approaches.** Have simple programs specific for the individual instrument written as macros in a matlab-type language, so that each use can adapt it to his specific needs...”

“**Don't waste too much time** making GUIs with all the bells and whistles.... “



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Graphics Publication quality?

“it should give an option to prepare final illustrations for publication...”

“Good quality vector graphics output in final analysis (eps or pdf)...”

“Good graph plotting to publication standards that is not too difficult to use (some "good" packages are quite opaque to the novice)...”



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Standards Data format

“The first important step is to establish a ***general file format*** with associated cross platform reading and writing routines...”

“...use consensus standard for file transfer (**NeXus**)”

“Input of data from multiple sources (x-ray and neutron)..”

“The ability to accept both x-ray and neutron data so that near unique models can be obtained when the techniques only vary by radiation!”

“A logical and comprehensive data file format that is the same across facilities. This would enable the growth of cross institutional analysis packages specialized for neutron scattering...”

“portability of data formats and software...”



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Standards Software tools

“***Uniform data analysis*** would make the analysis of NS data much easier, and probably more accurate...”

“Standardization between facilities and between instruments at a facility”

“Would like to see an ***industry wide*** set of tools available...”

“For data visualisation and reduction there should be a standard used World wide. i.e. Order of correction when converting from 2-D to 1-D data. The standard should be correct the 2-D data first then convert to 1-D. “

standard data fitting procedures should be there and correct error bars treatment is necessary



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Collaborate With whom?

“...check for possible collaborative ventures to leverage your resources;..”

“International Collaboration on this issue is important...”

“I think that is worth while but it is a major undertaking that is probably best done in **shareware** mode...”

“cooperation between communities...”

“...define an efficient general data format. NEXUS may be the answer but needs some updating. This can be done in collaboration with NIST and SNS in the US.”

“I believe the NIST analysis software should be the standard with continual improvements. ie. It is limited at the



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Collaborate With whom?

“...most of the facilities do not have enough people working on visualisation, reduction and analysis software.”

“Having sufficient budget and programmatic emphasis...”

“APPROPRIATE RESOURCING..”



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Delivery methods

Web or local? Open or closed?

“**portability...**”

“...available via **INTERNET** or be available free of charge...”

“Ease of access... “

“It is highly desirable to have **full access** to the facilities programs **from ones home institution...**”

“I much prefer to analyse data on a **laptop** anywhere (at home, at home institute or any other place)...”

“Make **source code freely available....** “

“... the beam scientists should be experienced with it, so they can help the users...”



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Delivery methods Open or closed?

“Use commercial software (Igor, Mathematica, IDL, MatLab, CrystalMaker, etc) with plugins made at facilities or elsewhere. A few commercial software are so good that a minimum development is required...” “...packages such as **IDL and MATLAB** are so powerful now that it is fast to develop the basic fitting and plotting routines needed.”

“Works on Unix (MacOS or Linux - no virus,etc), commercial software with good support (which is really the case for Igor, Mathematica and CrystalMaker) running on a laptop..”

“We need to use a **DCOM, .NET, or web-services** enabled solution. This would make things very easy...”



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Documentation

- “Up-to-date manuals with **good examples**... good and transparent manuals (or help files, but usually manuals are essential)...”
- “Higher quality documentation often required, users need to **understand the process** by which the data is reduced, what the parameters are, which they can adjust and whether they should do so. These should be as few as possible as you need to get the data in a final reduced form as quickly as possible if you are going to work with it to direct the course of an ongoing experiment...”
- “must have **online help** manual with a **tutorial** of the basic functions (plotting, fitting etc) to enable self education...”
- “The best is if software is written such that its use is self-explanatory, and there should be a manual...”



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Design and architecture

“There is often no **propagation of sample environment variables through data reduction software**, if you measure as function of field or temperature you will eventually want to plot against these variables, it is a major fiddle to have to extract all these variables from log files etc and get them matched up with integrated intensities...”

“...speed of data acquisition is increasing.
Increasing need to rapidly visualize and reduce data on the experiment and after for publication!!”



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Pitfalls

“Can’t please everybody...”

“...avoid the obvious kluge solutions.”

“The support is essential. Without permanent support, a software die...”



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Pitfalls

“If you attempt to combine (data collection, primary data reduction with limited visualisation, data analysis, and data visualisation) into one all-embracing package I'm afraid you will fail!...”

“Unfortunately, software developed by an IT-support group often fail...”

“The complete flexibility is handy. To compete with a dedicated package requires a serious professional programming effort...”