Computers and computing

Since the previous edition of the Yellow Book (1988), computing, like instrumentation, has undergone a revolution. The processing power, memory and disk space of the central VAX machines in 1988 are now easily surpassed by cheap laptop computers. Accordingly the role of computers in performing experiments at the ILL and analysing data has evolved considerably. However, one piece of advice for visiting scientists remains the same; the local contact is the first person to consult on issues relating to computing and, if necessary, he or she will direct you to one of the relevant services or groups.

Computing-related groups at the ILL

A user may need to consult one of three groups with respect to computing during or prior to an experiment at the ILL. The "Informatics Service" (SI, http: //dpt.ill.fr/SI/welcome.html) is responsible for much of the computing related infrastructure (network, email servers etc.) at the ILL. In particular the SI installs and maintains the data analysis computers on instruments. These are currently PCs running Windows or Linux. The SI also provides a visitor network for use with laptop computers.

The "Instrument Control Service" (SCI, http://dpt.ill.fr/SCI/sci_web3/index.html) is responsible for the electronics and basic data acquisition software. The current instrument control software (ICS), known as MAD, is being completely re-written in a modern, object-oriented language, with a view to offering easier maintenance, a simpler interface to the instrument and the possibility for the instrument scientist and users to write their own "intelligent acquisition sequences" to optimise the use of beamtime.

The Computing for Science group (CS, http://www.ill.fr/Computing) offers support to ILL scientists to provide the appropriate data analysis software. Otherwise CS explores the use of rapidly evolving computing resources to help optimise the use of beamtime in experiments at the ILL. In recent years this has entailed providing a web-server (http://barns.ill.fr) for access to raw data and analysis programs from outside the ILL (and its firewall), developing intelligent instrument set-up and experiment control software and applying the huge computational power currently available to numerical simulations of instruments and samples (e.g. molecular dynamics simulations).

Data analysis software

In terms of data analysis, the situation has changed completely since Fortran programs were run on central computers. While many Fortran programs still exist, and these have the advantage of having been debugged over many years, much recent development has used high-level languages like Matlab and IDL, which combine comprehensive libraries of mathematical functions with high quality graphics and the possibility of constructing graphical user interfaces (GUIs). In addition, over the years, a huge range of software has been developed, or simply arrived at the ILL, to cover the needs of a wide variety of experiments. The instrument scientists and local contacts know which software is most appropriate for an instrument and the experiment being performed. Only some of this software is developed and maintained by CS. While faster network connections make working remotely on ILL computers a possiblity, the most comfortable solution involves having the raw data and data analysis software on computers at home. The source codes of almost all ILL programs can be downloaded and, in cases where expensive compilers are needed (e.g. IDL for the LAMP program), it is also possible to obtain runtime executables (see ftp://ftp.ill.fr/pub/cs for programs maintained by CS).

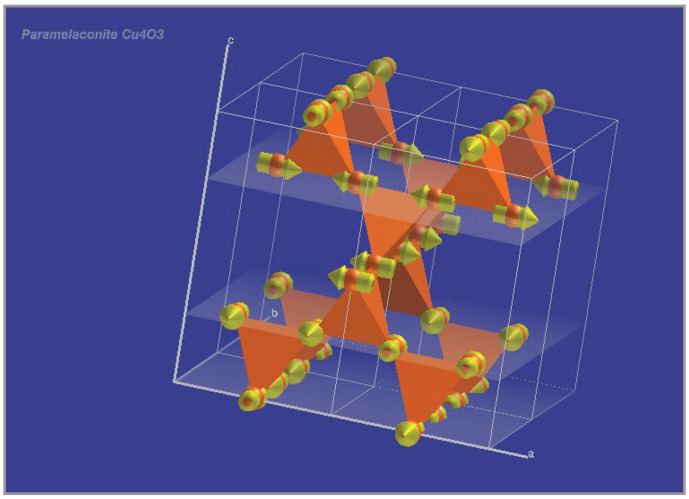
Transfer of data

All data is stored on a central server (Serdon) and is accessible from Unix and Linux computers in the directory /usr/illdata/'cycle', where 'cycle'='data' for the current cycle, 'data-1' for the previous cycle and, for example, 022 for the second cycle in 2002. Raw data can be transferred home

during an experiment by 'ftp' or 'scp'. Alternatively, on most data analysis computers it is possible to burn a CD with the data from an experiment. Direct access to all ILL data since the restart in 1995 is available via the BARNS web server and the Internet Data Access (IDA) utility.

New perspectives for computing at the ILL

Current computing power opens up a number of perspectives for optimising the use of neutron beamtime at the ILL.
By fitting data on-line (as it is measured) and integrating these results into decision-making during the data acquisition sequence, an "intelligent" sequence of scans can be performed. To date a number of instruments have used IDL based software (GEORGE or LIGHT) combined with the MAD ICS to simplify instrument setting-up, where this entails a sequence of scans to be performed. On D17 for example, rocking curves are performed in between acquisition scans to ensure that the sample is ideally located in the beam. On SANS and TOF machines, there have been examples of acquisition sequences in which individual scans are stopped after measured statistics or fit parameters have reached a certain precision. Some of this functionality will be included in the new ICS, while IDL and Matlab programs coupled to the ICS will continue to allow "intelligent" scan sequences to be instigated, in which scans are stopped according to predefined conditions based on numerical analysis.
Neutrons measure the structure and dynamics of condensed matter systems, but these properties are governed by potential and kinetic energy. Total energy calculations can be performed based either on empirical force fields or on parameter-free quantum chemistry techniques. Traditionally such methods have required high performance computing facilities, but nowadays, personal computers (and modest clusters) offer the possibility of studying models of the real system being investigated in the experiment in a reasonable time. In the case of complex systems for which the data cannot provide unequivocal evidence for a particular physical phenomenon, energy based simulations can offer independent evidence. In recent years a number of studies have been performed by ILL thesis students and scientists, ranging from molecular dynamics simulations of molecular glasses and biomolecules, through Monte Carlo simulations of adsorption in zeolites and carbon nanotube structures, to calculations of spin density and magnetic interactions using density functional theory-based, quantum chemistry methods. More details can be found at http://www.ill.fr/Computing/club.html and in recent ILL Annual Reports.
For a number of years ray-tracing simulations have been used to calculate neutron trajectories in neutron optical devices, such as guides and monochromators, and in other elements of instruments, like velocity selectors, allowing the design of guides and instruments to be optimised (see http://www.ill.fr/tas/mcstas). By combining such instrument simulations with accurate sample simulations and even experiment control software, virtual experiments will soon become a reality, allowing virtual training of users, checking the feasability of an experiment in terms of flux and resolution, optimising a measurement strategy prior to an experiment and separating sample and instrument related signals in the measured data.



Representation of a magnetic structure in LAMP.