Project Name: Automating the Chemical Crystallography experiment

Name of pipeline: X-Tray

Author information: Simon Coles

Current Status: Aspects implemented, full package not released

Purpose

To provide an automated and Grid-enabled environment for Service crystallography in the chemistry domain. The NCS Chemical Crystallography pipeline is designed to allow users to remotely access the service, monitor the progress of their sample through the system, steer various aspects of the experiment and download results.

High Level Description

The data collection and structure solution pipeline is defined by Python scripts, which use routines in legacy diffractometer control software, public domain structure solution, refinement and visualisation software and an in-house GUI. The remote user interface for the service aspects of the project is via a Web Services approach delivered through PHP. Existing programs which have been incorporated into this framework are:

COLLECT; A Python library of diffractometer control software
SHELXS/L; Public domain structure solution and refinement software
SYSTEM-S; Space group determination software
ORTEP3; Thermal ellipsoid plotting software

Decision Making

Decision making is performed at a number of points in the pipeline:

- Initial assessment of diffraction quality
- Accepting unit cell solutions
- Data collection resolution and exposure time
- Space group assignment
- Structure solution quality
- Atom typing
- Atom hybridisation
- Final refinement

Data Standards and Management

Data collection and structure solution parts of the overall pipeline are self contained and as such information is not exchanged. Current work is putting this part of the pipeline into the context of the whole experiment and therefore data management is currently being addressed

Languages

Developed in Python, PHP & Fortran.

External dependencies

None

Context/Audience/Environment

The automated structure solution and refinement system is primarily designed to work in-house on a personal computer. The whole NCS Grid Service is designed to be platform independent and allow any user (from novice to expert) to access the service and interact with their experiment.

Links to Supporting Documents

http://www.combechem.org
http://www.soton.ac.uk/~xservice

References

Powerpoint slides from a 1 week long workshop on eScience in Chemical Crystallography http://eprints.soton.ac.uk/9777/
PDF of talk on demonstration project (ECSES): http://eprints.soton.ac.uk/346/
Poster (BCA Spring Meeting 2003) on architecture: http://eprints.soton.ac.uk/7804/
Open Archive publishing talk at All Hands eScience meeting (2004) http://eprints.soton.ac.uk/8183/
Various other talks of interest: http://eprints.soton.ac.uk/11063/ ; http://eprints.soton.ac.uk/11259/ ; http://eprints.soton.ac.uk/12461/ ; http://eprints.soton.ac.uk/11240/