conference abstracts

s7.m3.o3 **The Genetic Diversity of available Crystallographic software freely obtainable via the internet.** L.M.D. Cranswick, *Collaborative Computational Project No 14 (CCP14) for Single Crystal and Powder Diffraction, Daresbury Laboratory, Warrington, WA4 4AD U.K, E-mail:L.Cranswick@dl.ac.uk, WWW http://www.ccp14.ac.uk*
Keywords: software, single crystal, powder diffraction.

Many full time and part time crystallographers are content in using a very limited set of analytical software. However, the option of applying other programs may assist in resolving stubborn problems involving non-typical structures. There is a wide variety of independent crystallographic software for single crystal and powder diffraction that is freely available off the internet. This includes a range of peak profiling, powder indexing, unit-cell refinement, single crystal structure solution, single crystal refinement, Rietveld refinement, structure checking, and visualization programs. As scientists are most at risk of "not knowing that they do not know", this presentations will quickly go through the various software options available to hopefully interest crystallographers in taking the time to look around at the range of available crystallographic software programs. Matching crystallographic software to the problem at hand can assist in overcoming what might seem the insolvable when using a limited suite of programs. Much of this software is mirrored and freely available via the CCP14 Project web site at http://www.ccp14.ac.uk

s7.m3.o4 **Maud: a Rietveld analysis program designed for the internet and experiment integration**. L. Lutterotti, *Dipartimento di Ingegneria dei Materiali, Università degli Studi di Trento, 38050 Trento, Italy*
Keywords: instrumentation, remote experimental control.

Maud is a Rietveld base analysis program written in Java for global analysis of diffraction spectra. Main goal is focused on crystal structure, quantitative phase, microstructure, texture and residual stresses simultaneous analysis. The ambitious results could be achieved only by a close integration with the experimental apparatus in a expert system like fashion. Texture and residual stresses analysis require the collection of several spectra and the analysis result and measurement time strongly depend on a correct choice of the experimental setting and conditions that in most cases should be refined during the analysis.

Due to the Java implementation the program may easily drive the experiment also remotely over the internet. Again the user may run it locally as an application or over the internet inside a browser as an applet. The second choice is more suited for a multi-user situation where the system manager could maintain just only one installation base that can be easily upgraded. Another advantage arises from the fact that applets run locally on the client not overloading the server. The program use also a distributed programming and threading technique to speed up the computation and share more memory between different machines when available.

The program is structured in a plug-in fashion; so, it will be easy to extend some features without recompiling it, but just adding a new module. One of the extensions is the interface with a specific data collection program to control the experiment progress as an expert system. In principle different instruments can be controlled by changing the remote control interface plug-in.