percentage of different kinds of secondary structure elements. The most extensive queries are those based on patterns of amino acid properties. It is possible to search for patterns combing such properties as environmental exposure, hydrophobicity, volume, polarity, isoelectric point, B values and so on. By taking properties from a given primary sequence and applying appropriate thresholds threading is possible. Alternatively, the starting properties can be taken from a known structure and structure similarity determined. A range of graphical tools can be applied to structures found in querying. These include plots of various property patterns, contact maps and 3-D images. The database system can be obtained by contacting the first author.

[1] I.N Shindyalov and P.E.Bourne (1995), J. App. Cryst. 28(6) 847-852.

MS03.02.04 A UNIVERSAL DATA EXCHANGE FORMAT FOR CRYSTALLOGRAPHY. B. McMahon, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England

The Crystallographic Information File (CIF) (Hall, Allen & Brown, 1991) is now the common exchange mechanism for crystallographic data supported by the IUCr. Increasingly, crystallographic program packages are able to read, write and validate CIF data. The file format has a simple syntactic structure, uses the ASCII character set for maximum portability between operating platforms, and is simply extensible. Dictionaries of recognised data names are constructed in a machine-readable formalism, allowing data relationships to be built and validated automatically.

This presentation will describe many current CIF applications, and discuss some of the considerations for successful programming of CIF software. There will also be a demonstration of how the IUCr uses standard software packages to check the quality of crystallographic data reported in its journals.

References
Hall, S. R., Allen, F. H. & Brown, I. D. (1991). *Acta Cryst.* A47, 655-685.

MS03.02.05 SIRWARE by G. Cascarano[+], A. Altomare[+], C. Giacovazzo[+], A. Guagliardi[+], A.G.G. Moliterni[+], D. Siliqi[+], M.C. Burla[*], G. Polidori[*] & M. Camalli[°] [+]Istituto di Ricerca per lo Sviluppo di Metodologie Cristallografiche - CNR c/o Dipartimento Geomineralogico - Campus Universitario Via E. Orabona, 4 - 70125 Bari - Italy.[*]Dipartimento di Scienze della Terra, Universita, 06100 Perugia, Italy. [°]CNR,Istituto di Strutturistica Chimica G. Giacomello, C.P.10, 00016 Monterotondo Stazione (RM), Italy.

New releases of our software and new programs will be presented. The covered fields are:
- treatment of powder data
A new integrated software based on EXTRA and SIRPOW exploiting all the synergies betweeen extraction intensities step and the Direct Methods application.
- single crystal
The new version of the Direct Methods program SIR (SIR96) including the treatment of electron diffraction data.
- protein data
A new program based on the integration of Direct Methods and isomorphous derivative techniques, solvent flattening and histogram matching.
A powerful and effective graphic interface is available in this software, suitable for all common platforms.
The programs will be free of charge for academic institutions.

MS03.02.06 COMPUTATIONAL ASPECTS OF XD. T. Richter, Institute for Crystallography, Free University of Berlin, Germany, T. Koritsanszky, S. Howard, P.R. Mallinson, Z. Su, N.K. Hansen

XD is a computer program package for multipole refinement and analysis of electron densities from diffraction data. It has been developed within an IUCr project by an iternational programing team. The main task of the package is to extract electronic properties from Bragg reflections and to perform topological analysis on 3D properties such as the electron density, its Laplacian function /1/ and the electrostatic potential. The package consists of the following programs:
- XDINI - convert data from conventional packages
- XDEDIT - edit master input file
- XDLSM - least squares program
- XDFOUR - general plane fourier program
- XDFFT - fast-fourier program
- XDPROP - electronic properties, topological analysis
- XDGEOM - geometrical analysis
- XDSTAT - statistical analysis
- XDVIB - thermal motion analysis
- XDGRAPH - graphical output
These programs will be described and their main computational aspects discussed.

/1/ R.F.W. Bader, Atoms in Molecules: A Quantum Theory, Oxford University Press (1990).

MS03.02.07 PARAMETERISING WEAK INTERACTIONS. S.J. Maginn, Molecular Simulations, 240/250 The Quorum, Barnwell Rd., Cambridge CB5 8RE, UK G.R. Desiraju, Dept. of Chemistry, University of Hyderabad, Hyderabad 500134, India

Forcefield parameters to account for a range of so-called "weak" interactions, such as C-H....O, have been successfully derived and tested.

Many crystal structures depend for their integrity on one or more of a range of so-called "weak" interactions. Examples of these include C-H....O, C-H....N, N....Cl etc.

No currently widely available molecular mechanics forcefield contains parameters to account for these interactions. Consequently, this is a weakness of the emerging forcefield-based crystal structure prediction methodologies (e.g. those of Gavezzotti *(1)*, and Karfunkel and Gdanitz *(2)*) - using such forcefields, structures containing "weak" interactions can never be accurately predicted.

A range of crystal structures containing C-H....O and C-H....N interactions has been used, along with the tools in the Cerius2 molecular modelling suite (such as molecular mechanics minimisation, and the Karfunkel and Gdanitz structure prediction method) *(3)*, to produce a customised forcefield which accounts for these, and which it is hoped will lead to more accurate structure predictions in future.

(1) A. Gavezzotti; J. Am. Chem. Soc. 113 (1991), p4622
(2) H.R. Karfunkel, R.J. Gdanitz; J. Comp. Chem. 13 (1992), p1171
(3) Cerius2, from Molecular Simulations Inc., 9685 Scranton Rd., San Diego, CA 92121-3752, USA, or 240/250 The Quorum, Barnwell Rd., Cambridge CB5 8RE, UK