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After about eight years of very active development, the Computational Crystallography Toolbox (cctbx) has evolved into a large collection of reusable, open source libraries covering many aspects of crystallography. The cctbx has roots in both small-molecule crystallography and macro-molecular crystallography and is used in both fields. The cctbx libraries are organized in a hierarchy of modules. It is possible to use subsets of the modules independently of other modules that may not be required for certain applications. We will present an overview of the cctbx architecture and the underlying software technology that has enabled the sustained growth of the libraries.
Links: cctbx.sourceforge.net, phenix-online.org

Keywords: crystallographic algorithms, object-oriented libraries, open source

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Identifying residues using 3D coordinates: An application of multiple APIs

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Given a small macromolecule of known sequence and the 3D atomic coordinates and atom types (but not the residue types) of all atoms, how should one assign the atoms to particular residues? This is a non-trivial structural homology problem. The Kabsch algorithm [1] can align structures of similar size, but it is not applicable when matching a small number of atoms from a residue template to a macromolecule. One could use the atoms to generate density and then trace the chain, but that fails to make use of the known information on atom types and requires a large complex program. We propose an alternate, simpler solution using a combination of CBFlib[2] and a linear algebra API to fit the molecule residue-by-residue starting with the largest and back-tracking when necessary. This approach to the problem is workable and suitable for embedding in graphics software. We created a program that uses these two APIs and in most cases identifies which atoms of a molecule belong to the specified residue types and produces a valid mmCIF file. Some issues that arose were variations in residue conformation, missing atoms and the similarity between the structure of some smaller residues to portions of other residues. The resulting program successfully assigns most of the test molecule atoms to the correct residues. The functionality of the program is being added to RasMol and PyMol.
[1] Kabsch, W. (1978). Acta Cryst. A34, 827-828.
[2] Bernstein, H. J., Ellis, P. J. (2005). Chapter 5.6 in "International Tables For Crystallography, Volume G: Definition and exchange of crystallographic data," Vol. G, S. R. Hall and B. McMahon, eds., International Union of Crystallography, Heidelberg: Springer, pp. 544 - 556.
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Keywords: structural homology, CBFlib, PDB

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Magnetic structure determination combining nonpolarised and polarised neutron diffraction

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Determination of the ground state is a key starting point in studying static and dynamic properties of any system: quantum magnet, multiferroic, heavy fermion, superconductor. For complex magnetic structures a combination of several techniques often is necessary to derive the unique solution. I will present a number examples from frustrated magnets ($Cu_2Te_2O_5Cl_2$[1] and Cu3TeO6) and quadrupolar ordered systems (CeB_6[2], $Ce_2Pd_{20}Ge_6$) which demonstrate usefulness of combination of nonpolarised and polarised neutron single crystal diffraction. This complex task is made possible using the Cambridge Crystallographic Subroutine Library[3].
[1] O.Zaharko et al. PRB 73,064422(2006)
[2] O.Zaharko et al. PRB 68,214401(2003)
[3] J.Brown http://www.ill.eu/sites/ccsl/html/ccsldoc.html

Keywords: magnetic structures, neutron polarimetry, frustrated magnets, quadrupolar ordering

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An algorithm for determining crystal lattices in unknown polycrystalline compounds

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When recovering crystallographic orientations of individual grains in polycrystalline materials both unit cell parameters and Bravais lattice are utilized. These crystallographic properties are normally determined from the radial spectra of diffraction rings by Powder Diffraction Indexing programs. Afterwards, grains are located in reciprocal space by identifying copies of the Bravais lattice [1,2]. Here, a new method is presented for determining the crystallographic properties of unknown polycrystalline compounds. Effectively, the method reduces the polycrystalline data set into a single crystal data set. As the Bravais lattice is embedded multiple times in the data set (multiplicity is given by number of grains) the method seeks to recover the base lattice by rotating the whole data set and match it against itself. If, by chance, the rotation is close to the crystallographic mis-orientation between two grains the algorithm identifies the two lattices. A match against previously identified lattice solutions is made. Clearly, the probability of making a false match in either selection step is high. In the algorithm a number of filtering steps ensures that the final estimation of the base lattice is only constructed from high frequency lattice points. The unit cell and Bravais lattice can then be determined from the base lattice by a single crystal indexing program. The algorithm itself is implemented in [2]. The algorithm and results will be presented.
[1] J. Wright, http://fable.wiki.sourceforge.net/imaged11
[2] S. Schmidt, http://fable.wiki.sourceforge.net/GrainSpotter

Keywords: pattern recognition, indexing, polycrystals