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TOPAS - programming ideas

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X-ray diffraction analysis is a hands-on process with many preliminary computations necessary before achieving an acceptable level of completeness; this interactive analysis drives the need for computational speed and program flexibility. With the arrival of fast computers simple Rietveld [1] refinements have become trivial with refinements taking as little as 0.1 seconds. Increased computing speed however has also led to ambitious simultaneous analysis of hundreds or even thousands of diffraction patterns; thus maintaining computational speed whilst conserving memory usage continues to be of paramount importance. More recent powder diffraction areas such as Pair Distribution Function and Stacking Fault analyses are similarly computationally demanding and interactive. These demands have led users to favor fast, flexible and relatively easy to use software. This talk focuses on the techniques used in the program TOPAS [2] [3]; it includes the use of tree like internal data structures, the use of computer algebra for abstract communication between data nodes and the use of an interrupt driven logic flow that hides underlying complexity. Of importance is the use of a programming language that allows the implementation of these ideas in a speedy manner; the language of choice being c++.

[1] Rietveld, H.M. (1969). J. Appl. Cryst., 2, 65-71.
[2] Coelho, A. A. (2017). TOPAS Academic. Version 6. http://www.topas-academic.net
[3] Bruker (2017). TOPAS. Version 6.0. Bruker AXS, Karlsruhe, Germany

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