TOPAS – A program for analysing X-ray diffraction data

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TOPAS [1][2] is a computer program that brings the areas of computer programming, mathematics and the science of diffraction analysis together to form a comprehensive X-ray diffraction analysis package. Both computational speed and program flexibility is of great benefit. Routine Rietveld [3] refinements are trivially performed today 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; computational speed therefore 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. This talk focuses on the techniques used in TOPAS to accommodate these demands; 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++. Complying with c++ standards allows for easy compilation on Cloud computing platforms, such as Amazon EC2, bringing supercomputing capabilities to the desktop.

[1] Coelho, A. A. (2018). J. Appl. Cryst. ***51****, 210-218. "TOPAS & TOPAS-Academic: An optimization program integrating computer algebra and crystallographic objects written in c++"*

[2] Bruker (2017). TOPAS. Version 6.0. Bruker AXS, Karlsruhe, Germany

[3] Rietveld, H.M. (1969): A profile refinement method for nuclear and magnetic structures. J. Appl. Cryst., ***2****, 65-71.*

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