New features and enhancements in TOPAS Version 8

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Version 8 of TOPAS and its academic variant TOPAS-Academic [1] is a substantial expansion of computational performance, scalability, and automation capabilities designed for industrial, synchrotron, and high-throughput environments. A key enhancement is the ability to run large refinements, particularly those involving extensive memory usage or thousands of iterations. A new A-matrix handling method, including sparse storage and automatic zero-element enforcement, improves the BFGS approximation and significantly increases convergence stability in refinements containing hundreds of thousands of independent parameters. Version 8 also introduces peak-stretching functionality, enabling rapid approximation of peak shapes without recalculating full convolution buffers, yielding substantial speed gains in multi-phase or computed-tomography refinements. Large-scale refinements also benefit from reuse of objects across thousands of phases or datasets; these reusable objects include lattice parameters, structure details, phase definitions, peak buffers, and structure-factors. This dramatically reduces memory usage and derivative computation time, enabling refinements involving 150,000+ structures and thousands of diffraction patterns to complete within minutes on standard hardware.

Version 8 also introduces energy minimization and molecular dynamics strategies. This includes reporting on the Madelung constant, the Coulomb potential at a site, and the application of a force on a site.

The GUI now incorporates refinement of ADP parameters; the generation of Pair Distribution Functions (PDF) and refinement of the PDF from within the GUI. PDF refinement now includes refinement of ADP parameters as well as graphical display of partial PDFs. In Rietveld refinement, improvements in Graphical display include enhanced handling of HKL tick marks in 2D and 3D surface graphics and the ability to select files for display using grep.

[1] A. A. Coelho, J. Appl. Cryst. (2018). 51, 210-218