Computer Software, *Powder Diffraction*, and Science

Diffraction seems to be ahead of the curve so often. Our community was one of the first to make use of digital computers, and in fact crystallographers were important in the development of the first and still important computer language, Fortran. We continue to lead to this day: so very few fields can *ever* claim to fit realistic physical/chemical models to their data via first-principles computations, but in the pages of this Journal, this is routine practice.

Communication of electronic data in science is also a forefront topic. Astronomers, aided by the fact that they all observe the same sky, have developed a standardized way to exchange their observations. They are exemplary for their amazing system that allows everyone to access these observations. Our field has gone one step farther with standardization, though. With the Crystallographic Information Framework (CIF) we have a way to exchange not only our observations, but also our results as well. Other fields are just beginning to tackle how this should be attempted, but in this issue we can see how CIF is being put to work by the ICDD for submission of data and results to their Powder Diffraction File database [Sagnella LINK/PAGE].

We all know that computation has evolved. For years I have had a phone with greater memory and speed than the single computer that served Rutgers University and State of New Jersey's educational computing center, where I first analyzed diffraction data (with computer cards and at a cost of hundreds of dollars for each hour of computation). No longer is the cost or availability of computer hardware a limiting factor. For most purposes, a laptop is all that is ever needed – although big screens are so very nice.

Computers may be abundant, but good scientific software is not. Lack of software continues to limit what data we can analyze, how we perform our studies and how much expertise (and effort) it takes to get them done. For this reason, we periodically review progress in powder diffraction software. This is the second special issue of this Journal devoted to software. Herein we have eight articles on different aspects of computing for powder diffraction. Thanks go to the authors who clearly put much time into writing code that benefits us so richly, as well as communicating their work to us. Our community owes so very much to people such as Daniel Louër and Ali Boultif, who here describe the latest version of their pioneering autoindexing program, DICVOL [Louer LINK/PAGE]. This is the latest from this group in a series of contributions that goes back over 40+ years and has enabled a huge amount of science.

Software is even changing the way that scientists write papers, as evidenced herein. In recent years I have become a strong partisan for using the Python computer language in science and wanted to include an introductory article on it here, but written from a wider perspective than my own [Ayers LINK/PAGE]. I invited two software engineers to collaborate. For our writing we used tools designed primarily for collaboration on software creation and bug tracking, and, in contrast to my previous experience with collaborative writing, there was no exchange of paper documents, no face-to-face discussions and not even any phone calls. I have yet to ever meet or even speak with either of these coauthors.

Computers indeed have changed how science is done.

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