The evolution of crystallographic software tools and their efficacy in teaching endeavours

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In single-crystal structure determination, instrumentation and user-friendly software and tools for collecting data, then solving, model-building and refining crystal structures have advanced tremendously over the last 40 years; way beyond what one could have imagined back then. Utilising hardware or data to its full potential requires good software to go with it and good software requires good computing resources. For the newest generation of enthusiastic crystallographers, the mouse click and smart graphical use interfaces (GUIs) are ubiquitous and it is perhaps hard to imagine what pre-mouse computing looked like: paper tapes and teletypes, punch cards, magnetic tapes, mainframes, toggle-switches to boot computers, line commands, and walking down the road to pick up line-printer output – things one still did in the early 1980s. Crystallographers of that time often needed some programming skills, too, because one often had to have small routines to process and reformat data or output for use in the next step of the workflow. The advent of desktop PCs in the 1980s opened the way to cheaper, accessible, easier to use and more standardised operating systems. This allowed crystallographic software to develop in parallel with the evolution of the functionality of computer hardware, operating systems, graphics capabilities and the dramatic increase in computing speed. Today's users now have access to impressive GUIs and extensive functionality.

Software development requires people and good ideas. While some excellent software has been developed commercially, some of our most indispensable software has been developed completely voluntarily and the community has been most fortunate to benefit from the ongoing dedication of such enthusiasts.

Teaching the concepts and practice of crystallography to newcomers to the field is an important endeavour too. As an example, symmetry concepts are sometimes difficult for students to visualise. While traditional physical models and drawings are still valuable, the opportunities provided by good, interactive graphics depictions are indispensable. The tools available in today's software allow tutors, with just few mouse-clicks, to show their students how to extract much more information about the structure than was readily accessible earlier, such as rotatable 3D maps of residual electron density, or to easily model disorder and utilise and other features that help validate the developed model or suggest aspects requiring further attention, while allowing answers to be sought to questions that were perhaps unanswerable some years earlier.

This presentation will take a journey through the evolution of crystallographic software tools and look at some examples of where today's tools are useful in demonstrating and teaching the concepts of crystallography at various levels.