# International Union of Crystallography Computing Schools

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## Abstract

*Reminiscences on IUCr Computing Schools and their place in the overall scheme of the universe.*

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I am riding on a limited express, one
of the crack trains of the nation.
Hurtling across the prairie into blue
haze and dark air go fifteen all-steel
cars holding a thousand people.
(All the coaches shall be scrap and
rust
and all the men and women laughing in
the diners and sleepers shall pass to
ashes.)
I ask a man in the smoker where he is
going and he answers: "Omaha[1]."
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I quote Sandburg at this School for Crystallographic Computing, the thirteenth in a series of such schools organized under the auspices of the IUCr Commission on Crystallographic Computing, in order to evoke the emotional aspect of the work of the participants. The hurtling train can represent the incredible and continuing improvements that have occurred in our ability, over the last 50 years, to compute the results of the insights put forward by Laue, the Braggs, Ewald, and those who followed. It can also represent the collective effort of the many crystallographers and computer scientists and engineers; the men and women who have brought our ability to process automatically and calculate quickly results that were, 40 short years ago, so tantalizing and daunting.

It is surely true that each of us, when we participate in schools such as this one, take away information which directly contributes to the overall progress in crystallography. Without the wonderful machinery available to us, the understanding of the computations required, and the programs to drive the machinery, the "train" would be still standing in the station. To illustrate exactly what has happened in the last half-century, consider Figure 1 showing the number of macromolecular structures deposited with the PDB as a function of year.

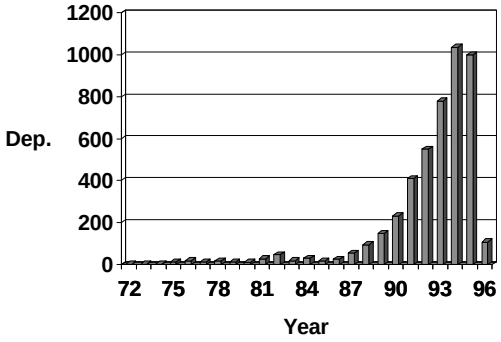


**Figure 1 Growth of the PDB. Data generated from *http://www.sdsc.edu/moose***

This productivity in our science has been partly fueled by the "stuff" of these IUCr schools. Each individual, while visiting "Omaha" enjoying the Old Market District of calculating first phases from MIR data, riding the Fremount Dinner Train, cutting into the tender steak of viewing a well fitted map, or indulging in one of the many other intellectual challenges which have kept the "Limited" rolling, does not dwell on scrap and rust. But of course the Second Law is with us - even as Sandburg sensed without benefit of J. W. Gibbs' insights. In order to illustrate this I have brought for your inspection the programming board from an IBM 407 accounting machine. This is a board that would store zero bits. You will note that it is much more substantial than the type of circuit boards you know and love. With this board in the machine, a pile of punched cards, and a collection of plug wires one could, in the course of a long night, carry out the Fourier transform of a two-dimensional projection. When I started in crystallography this was the great

night out in "Omaha." This is because, up to that time in the early fifties, the technology that we had was Beevers-Lipson strips and a "grind-em-up" Marchant gear-driven calculator. The strips, which are contained in the wooden box, I have brought here today for you to admire. These strips are still generated inside current FT computer codes. A tedious business it would appear, but I remember my post-doctoral mentor P. M. Harris, at The Ohio State University, saying what a boon they were compared to using a slide rule or regular trig tables. From this background you should be able to appreciate why I can be so thrilled when my obsolete $4k 1995 PC computes Fourier Transforms as quickly as the $M "super" computer I had the privilege of using just a few score months ago.

In examining the books[2-8] that resulted from past schools there is a good deal of scrap and rust to be seen, but there are also golden, incorruptible monuments to the progress we celebrate. The first school which I attended in 1969 was held in Ottawa. There the emphasis was on the details of specific programs for small molecules. There was a great deal on the mathematical basis for calculations of Fourier transforms, least-squares refinement, and the plotting of ball-and-stick models. There were also interesting presentations on the relative strength of ALGOL as a "higher" programming language. The beginning of programs for macromolecular calculations was presented by G. Kartha. In it he reported on a Fourier transform for ribonuclease at 2 Å resolution using ~9000 reflections to calculate a 60X88X100 grid. He reports 52 minutes on the IBM 7040, 17 min. on the IBM 7044, and the hope that it would drop to ~2 min. when the new CDC 6400 became available. For comparison: today an IBM 6000 workstation does the same grid with ~16000 reflections in 1.5 min. The spectacular improvement is in cost, not speed, for this routine operation. In addition to the carefully cost-accounted time, details of the allocation of memory were of concern. On these machines 192kBytes (6-bit bytes) was all that was available.

By the time of the IUCr school in Czechoslovakia in 1975 there was much more emphasis on solution and refinement. Small molecules still dominated, but macromolecular calculations were much more prominent in that school. There is much less about specific machines, since the numbers and kinds had increased dramatically by then. The "mini-computer" was then available and coming into use by crystallographic laboratories. A highlight of that time was the presentation on the use of the fast Fourier transform in crystallography.

At the conference in Holland in 1978 SHELX is described at an IUCr school for the first time and there is a whole session devoted to "Program Systems on Large Scale Computers" with a second session on mini-computers. At this school "micro-processors" are being touted for an other "first." This trend to smaller machines shows up again in the Bangalore school in 1980. But here the main emphasis is on methods of carrying out macromolecular crystallographic analysis starting with automated data collection and through all the steps to map interpretation. At that meeting Diamond predicted that hardware and software would soon be commonly available for interactive graphics.

The school moved back to Canada in 1981. One may then see the results of the most successful methods presented in the earlier schools coming into productive use. The improvements in hardware and its decrease in cost, the improvements in software, both optimizing compilers and crystallographic codes, are all evident in the presentations. There are reports on GRIP, FRODO, BUILDER, and GRAMPS under the category of "molecular manipulators and displays." Hardware, storage, and timing considerations have all but disappeared from the scene; it reads as if the "crystallographic age" had dawned.

In 1987 in Australia in addition to the "required courses" one finds some other interesting facets of crystallography featured: fiber and electron diffraction. In addition, a whole session on databases was presented. By this school the title of the book is made by adding a sequence number. Finally, in 1990 in France, one sees the ascendancy of macromolecular analysis. In addition to its sequence number the book has a subtitle of "From Chemistry to Biology." This school featured the basics through advanced methods and software for carrying out macromolecular crystallography; from data collection through structure analysis, modeling, and databases.

One can see that in the earliest schools crystallographers expended many happy nights in "Omaha" trying to figure out the best ways to conserve storage and optimize machine code. Be thankful now that the hardware and software is so fast and plentiful that these kinds of efforts are no longer of importance. Now we can focus on improved methods of phase determination, the most effective refinement strategy, and the "problems" of dealing with synchrotron data.

With Hamlet's[9] help I'll get off the scrap and rust heap:

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See you now.
Your bait of falsehood takes this carp
of truth.
And thus do we of wisdom and of reach,
With windlasses and with assays of
bias,
by indirection find directions out.
So by my former lecture and advice,
Shall you my son.
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Act II, scene I, line 62

The reason we are all here in Bellingham today is to find ever better ways to wind our windlasses and assay our biases. I feel sure that this week's participants, like those in schools past, will help keep "Crystallography Limited" hurtling into the next millennium. Your talent and energy will help to accomplish the work yet to be done.

## References


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[9] W. Shakespeare, "The Tragicall Historie of Hamlet, Prince of Denmarke" Newly imprinted and enlarged to almost as much again as it was according to the true and perfect coppie by I.R. For N. L. At his shoppe under St. Dunstan Church, London, 1604.